Curriculum Vitae

PERSONAL INFORMATION

- **Family name, First name:** **Liwo, Józef Adam**
- **ORCID ID:** **0000-0001-6942-2226**
- **Date of birth:** **15 April 1960**
- **Nationality:** **Polish**
- **URL for web site:** **http://www.liwo.strony.ug.edu.pl/**

PRIMARY RESEARCH

I am focused on determining the physical principles that make (bio)macromolecules and molecular assemblies attain and keep stable their unique three-dimensional structures. I use the coarse-grained approach (renormalization group theory) and statistical mechanics to relate atomistic-detailed interactions to net forces that govern molecular motion. I constructed the theory of and implemented in a large part the Unified Coarse-Grained Model for macromolecular simulations, which is probably the only physics-based coarse-grained model that is capable of predicting the structure of proteins and nucleic acids; part of the relevant software is available from www.unres.pl (downloadable standalone package) and http://unres-server.chem.ug.edu.pl (server version).

CURRENT POSITIONS

- **Full Professor and Head of Laboratory of Molecular Modeling**, Faculty of Chemistry, University of Gdańsk, Gdańsk, Poland.

EDUCATION, SCIENTIFIC DEGREES AND TITLES

2001 **Professor of Chemical Sciences** (title received from the President of the Republic of Poland after approval by the Central Committee for Scientific Degrees and Titles).

1997 **Habilitation** (Physical and Theoretical Chemistry) Faculty of Chemistry, University of Gdańsk, Poland. Thesis title: Design of an empirical force field and conformational-search methods for protein-structure prediction from amino-acid sequences

1989 **PhD** (Physical and Theoretical Chemistry) Faculty of Mathematics, Physics, and Chemistry Chemistry, University of Gdańsk, Poland. Thesis title: Theoretical analysis of the conformations and molecular fields of neurohypophyseal hormones - an attempt to structure-activity correlation, supervisor: Prof. Zbigniew Grzonka

1983 **MSc** (Chemistry, with honors) Faculty of Mathematics, Physics, and Chemistry, University of Gdańsk, Poland. The curriculum included extended program in math. Thesis title: A general method for the determination of the stoichiometry of complex chemical-equilibrium systems from physicochemical measurements, supervisor: Dr. Jurand Czerminski

PRE-DOCTORAL TRAINING

- III–VI.1987 **Short-term internship** in the Institute of Physics, Nicholas Copernicus University, Toruń, Poland (J.S. Kwiatkowski group).

POST-DOCTORAL TRAINING

- 1990–1992, 1994, **Postdoctoral Associate**, Department of Chemistry and Chemical Biology, Cornell University (supervisor: H.A. Scheraga).

EMPLOYMENT

- 1983–present **Faculty of Chemistry, University of Gdańsk**; tenured full professor since 2001; member of the Faculty Council since 1997; director of the Laboratory of Molecular Modeling since 1999.
- 2014–present **Korea Institute for Advanced Study (KIAS)**, Seoul, Republic of Korea; KIAS Scholar.
- 2003–2010 **Senior Research Associate, Dep. of Chemistry and Chemical Biology, Cornell University** (H.A. Scheraga group).
- 2001–2003 **Vice-Director for Scientific Affairs**, Academic Computer Center in Gdańsk, **TASK**.
- several short-term employments on the **visiting-scientist or visiting professor basis** (Cornell University (USA), Mt. Sinai School of Medicine (USA), SUNY Upstate Medical Center (USA), University of Uppsala (Sweden), Beijing Institute of Technology (P.R. China) in years 1993-2015.

ORGANIZATIONAL ACTIVITY

- 1998–present **Member of the Interdisciplinary Team** of Mathematical Modeling at the Academic Computer Center in Gdańsk, **TASK.**
- 1998–2001 **President of the Scientific Council** of the Academic Computer Center in Gdańsk, TASK.
- **Organizer and co-organizer** of 8 international **conferences** in the last 5 years:
  - CBSB14 meeting in Gdańsk (2014)
  - 1st Korean-Polish Conference on Protein Folding, Seoul, S. Korea (2015)
  - 2nd Polish-Korean Conference on Protein Folding, Gdańsk, Poland (2016)
  - 3rd Korean-Polish Conference on Protein Folding, Gohan, S. Korea (2017)
  - Workshop 'Physics and Biology of Proteins', Natal, Brazil (2017)
  - 4th Polish-Korean Conference on Protein Folding, Iława, Poland (2018).
  - 5th Korean-Polish Conference on Protein Folding, Seoul, S. Korea (2019)
  - 6th Polish-Korean Conference on Protein Folding, Jastrzębia Góra, Poland (2021)
  - 7th Korean-Polish Conference on Protein Folding, Seoul, S. Korea (2022)
  - 8th Polish-Korean Conference on Protein Folding, Jastrzębia Góra, Poland (2023)
  - Workshop on Mathematics and Computer Science in Modeling and Understanding of Structure and Dynamics of Biomolecules, Banff, Canada (2019)

PROFESSIONAL MEMBERSHIPS

- 2008–present Member of the American Chemical Society
- 2009–present Member of the Biophysical Society
- 2015–present Member of the Polish Chemical Society
- 2003–present Member of the Scientific Society of Gdańsk
- 2001–present Member of the Polish Society of Computer Simulation
- 2012–2015 Member of the Committee of Biochemistry and Biophysics of the Polish Academy of Sciences
- 2015–present: Member of the Polish Chemical Society.

EXPERT ACTIVITY

- **Reviewer of research grants** for the Polish National Science Centre (2012–present; earlier for the Polish Ministry of Science and Higher Education)
- **Reviewer of research grants** for Romanian and Czech grants agencies
- **Reviewer of computational grants** for Partnership of Advanced Computing in Europe (PRACE)
- **Member of the Council of Science**, Faculty of Chemistry, University of Gdańsk
- **Member of the Board** of Doctoral Procedures in Physical and Theoretical Chemistry, Faculty of Chemistry, University of Gdańsk
- **Reviewer of several academic position applications and promotions** for the Polish and U.S. academic institutions
- **Reviewer of more than 10 Ph.D. theses, more than 10 habilitation theses and 4 professor title applications** for the Polish Central Board for Scientific Degrees and Titles (CK), and member of the respective degree/title award boards
- **Reviewer of 30 papers yearly on average for international scientific journals** (J. Phys., Chem. B, Sci. Rep., J. Chem. Phys., Proteins: Struct. Func. Bioinf., etc.)
- **Member of the Interdisciplinary Team of Mathematical Modeling**, Academic Computer Center in Gdańsk, TASK.

HONORS AND AWARDS

2021 **Individual award** from the Minister of Education and Science
2019 **Special Award** from the Rector of the University of Gdańsk for outstanding scientific research
2016 **Medal** of the Polish Committee of National Education
2015 **Travel Award** from Biophysical Society (presented on 59th National Biophysical Society Meeting in Baltimore)
2013 **'Mistrz' (Master)** subsidy for distinguished professors from the Foundation for Polish Science
2013, 2006, 1999, 1993 **awards from the Rector** of the University of Gdansk for distinguished research
2012 **Elected as a member of the Committee** of Biochemistry and Biophysics of the Polish Academy of Sciences
2001, 1995, 1989 **Award as a team member** from the Polish Minister of Education
1998 **Individual award** from the Polish Minister of Education.

PUBLICATIONS

283 original papers published, 1 in press, and **10 review articles** in ISI journals, 6 original papers and 2 review articles in non-ISI journals, **13 book chapters**, **editor of 1 book**; 81 papers, 5 book chapters and 1 edited book in the last 10 years. Number of citations excluding self-citations: 6320. **H-index: 49**.

CURRENT RESEARCH SUPPORT (WITH ROLE AS PI)

"Data-assisted modeling of the ensemble structure of intrinsically disordered proteins and their assemblies", National Science Centre (NCN), grant contract number: UMO-2021/40/Q/ST4/00035, total budget: 1630572 PLN.

TEACHING

Present:

- 1 obligatory course (Theoretical Chemistry; course director) for M.Sc. students
- 2 courses for Chemistry majors (Numerical Methods in Chemistry and Programming in C and FORTRAN)
- 2 lectures for graduate students (Protein Structure and Energetics and Molecular Simulations in Chemistry).

In the past:

- General and Inorganic Chemistry lab and recitation classes (as T.A.)

- Informatics in Chemistry (lectures and lab classes)
- Molecular Modeling (lectures and lab classes).

▪ MENTORING

- Currently mentors 1 postdoc and 1 graduate student; 11 graduate students, 11 undergraduate students and 3 postdocs mentored in the past. 4 graduate students mentored in the past found academic positions, 4 graduate students mentored in the past (Adam Sieradzan and Magdalena Mozolewska and Agnieszka Lipska) received early-stage-researcher PRELUDIUM grants from the Polish National Science Centre (NCN) while doing Ph.D.

Józef Adam Liwo

List of publications and invited presentations

Original papers in ISI journals

283. A. G. Lipska, A. K. Sieradzan, S. Atmaca, C. Czaplewski, **A. Liwo**. Toward Consistent Physics-Based Modeling of Local Backbone Structures and Chirality Change of Proteins in Coarse-Grained Approaches. *J. Phys. Chem. Lett.*, **2023**, 14, 9824-9833.

282. L. Borges-Araújo, I. Patmanidis, A. P. Singh, L. H. S. Santos, A. K. Sieradzan, S. Vanni, C. Czaplewski, S. Pantano, W. Shinoda, L. Monticelli, Pragmatic Coarse-Graining of Proteins: Models and Applications. **A. Liwo**, S. J. Marrink, P. C. T. Souza. *J. Chem. Theory Comput.* **2023**, 19, 7112-7135.

281. A Danielsson, S. A. Samsonov, **A. Liwo**, A. K. Sieradzan. Extension of the SUGRES-1P Coarse-Grained Model of Polysaccharides to Heparin. *J. Chem. Theory Comput.*, **2023**, 19, 6023-6036.

280. M. F. Lensink, G. Brysbaert, N. Raouraoua, P. A. Bates, M. Giulini, R. V. Honorato, C. van Noort, J. M. C. Teixeira, A. M. J. J. Bonvin, R. Kong, H. Shi, X. Lu, S. Chang, J. Liu, Z. Guo, X. Chen, A. Morehead, R. S. Roy, T. Wu, N. Giri, F. Quadir, C. Chen, J. Cheng, C. A. Del Carpio, E. Ichiishi, L. A. Rodriguez-Lumbreras, J. Fernandez-Recio, A. Harmalkar, L.-S. Chu, S. Canner, R. Smanta, J. J. Gray, H. Li, P. Lin, J. He, H. Tao, S.-Y. Huang, J. Roel-Touris, B. Jimenez-Garcia, C. W. Christoffer, A. J. Jain, Y. Kagaya, H. Kannan, T. Nakamura, G. Terashi, J. C. Verburgt, Y. Zhang, Z. Zhang, H. Fujuta, M. Sekijima, D. Kihara, O. Khan, S. Kotelnikov, U. Ghani, D. Padhorny, D. Beglov, S. Vajda, D. Kozakov, S. S. Negi, T. Ricciardelli, D. Barradas-Bautista, Z. Cao, M. Chawla, L. Cavallo, R. Oliva, R. Yin, M. Cheung, J. D Guest, J. Lee, B. G. Pierce, B. Shor, T. Cohen, M. Halfon, D. Schneidman-Duhovny, S. Zhu, R. Yin, Y. Sun, Y. Shen, M. Maszota-Zieleniak, K. K. Bojarski, E. A. Lubecka, M. Marcisz, A. Danielsson, L. Dziadek, M. Gaardlos, A. Gieldon, **A. Liwo**, S. A. Samsonov, R. Slusarz, K. Zieba, A. K. Sieradzan, C. Czaplewski, S. Kobayashi, Y. Miyakawa, Y. Kiyota, M. Takeda-Shitaka, K. Olechnovic, L. Valancauskas, J. Dapkunas, C. Venclovas, B. Wallner, L. Yang, C. Hou, X. He, S. Guo, S. Jiang, X. Ma, R. Duan, L. Qui, X. Xu, X. Zou, S. Velankar, S. J. Wodak. Impact of AlphaFold on structure prediction of protein complexes: The CASP15-CAPRI experiment. *Proteins: Struct. Funct. Bioinf.*, **2023**, 91, 1658-1683.

279. M. Maszota-Zieleniak, **A. Liwo**, S. Ricard-Blum, S. A. Samsonov. Interplay of heparan sulfate chains with the core proteins of syndecans 2 and 4. *Proteoglycan Res.*, **2023**, 1, e10.

278. K. M. Ocetkiewicz, C. Czaplewski, H. Krawczyk, A. G. Lipska, **A. Liwo**, J. Proficz, A. K. Sieradzan, P. Czarnul. UNRES-GPU for Physics-Based Coarse-Grained Simulations of Protein Systems at Biological Time-and Size-Scales. *Bioinformatics*, **2023**, 39, btad391.

277. strains. A. G. Lipska, A. K. Sieradzan, C. Czaplewski, A. D. Lipińska, K. M. Ocetkiewicz, J. Proficz, P. Czarnul, H. Krawczyk, **A. Liwo**. Long-time scale simulations of virus-like particles from three human-norovirus *J. Comput. Chem.*, **2023**, 44, 1470-1483.

276. **A. Liwo**, M. Pyrka, C. Czaplewski, X. Peng, A. J. Niemi. Long-Time Dynamics of Selected Molecular-Motor Components Using a Physics-Based Coarse-Grained Approach. *Biomoecules*, **2023**, 13, 941.

275. A. K. Sieradzan, J. Sans-Duñó, E. A. Lubecka, C. Czaplewski, A. G. Lipska, H. Leszczyński, K. M. Ocetkiewicz, J. Proficz, P. Czarnul, H. Krawczyk, **A. Liwo**. Optimization of parallel implementation of UNRES package for coarse-grained simulations to treat large proteins. *J. Comput. Chem.*, **2023**, 44, 602-625.

274. S.-J. Chen, M. Hassan, R. L. Jernigan, K. Jia, D. Kihara, A. Kloczkowski, S. Kotelnikov, D. Kozakov, J. Liang, A. **Liwo**, S. Matysiak, J. Meller, C. Micheletti, J. C. Mitchell, S. Mondal, R. Nussinov, K.-i. Okazaki, D. Padhorny, J. Skolnick, T. R. Sosnick, G. Stan, I. Vakser, X. Zou, G. D. Rose. Protein folds vs. protein folding: Differing questions, different challenges. *Proc. Natl. Acad. Sci.*, **2023**, 120, e2214423119.

273. peptides. C. Schulze, A. Danielsson, **A. Liwo**, D. Huster, S. A. Samsonov, A. Penk. Ligand binding of interleukin-8: a comparison of glycosaminoglycans and acidic *Phys. Chem. Chem. Phys.*, **2023**, 25, 24930-24947.

272. R. Ślusarz, E. A. Lubecka, C. Czaplewski, **A. Liwo**. Improvements and new functionalities of UNRES server for coarse-grained modeling of protein structure, dynamics, and interactions. *Front. Mol. Biosci.*, **2022**, 9, 1071428.

271. E. A. Lubecka, **A. Liwo**. A coarse-grained approach to NMR-data-assisted modeling of protein structures. *J. Comput. Chem,*, **2022**, 43, 2047-2059.

270. C. Sikorska, **A. Liwo**. Origin of Correlations between Local Conformational States of Consecutive Amino Acid Residues and Their Role in Shaping Protein Structures and in Allostery *J. Phys. Chem. B*, **2022**, 126, 9493-9505.

269. I. Biskupek, C. Czaplewski, J. Sawicka, E. Iłowska, M. Dzierżyńska, S. Rodziewicz-Motowidło, A. Liwo. Prediction of Aggregation of Biologically-Active Peptides with the UNRES Coarse-Grained Model. *Biomolecules*, **2022**, 12, 1140.

268. I. Biskupek, A. Sieradzan, C. Czaplewski, A. **Liwo**, A. Lesner, A. Giełdoń. Theoretical investigation of the coronavirus SARS-CoV-2 (COVID-19) infection mechanism and selectivity. *Molecules*, **2022**, 2080.

267. M. Bogunia, A. **Liwo**, C. Czaplewski, J. Makowska, A. Giełdoń, M. Makowski. Influence of temperature and salt concentration on the hydrophobic interactions of adamantane and hexane. *J. Phys. Chem. B*, **2022**, 126, 634-642.

266. C. Czaplewski, Z. Gong, E.A. Lubecka, K. Xue, C. Tang, **A. Liwo**. Recent Developments in Data-Assisted Modeling of Flexible Proteins. *Front. Mol. Biosci.*, **2021**, 8, 765562.

265. **A. Liwo**, C. Czaplewski, A.K. Sieradzan, A.G. Lipska, S.A. Samsonov, R.K. Murarka. Theory and Practice of Coarse-Grained Molecular Dynamics of Biologically Important Systems. *Biomolecules*, **2021**, 11, 1347.

264. M.F. Lensink, G. Brysbaer, T. Mauri, N. Nadzirin, S. Velankar, R.A.G. Chaleil, T. Clarence, P.A. Bates, R. Kong, B. Liu, G. Yang, M. Liu, H. Shi, X. Lu, S. Chang, R.S. Roy, F. Quadir, J. Liu, J. Cheng, A. Antoniak, C. Czaplewski, A. Giełdoń, M. Kogut, A.G. Lipska, **A. Liwo**, E.A. Lubecka, M. Maszota-Zieleniak, A.K. Sieradzan, R. Ślusarz, P.A. Wesołowski, K. Zięba, C.A. Del Carpio Muñoz, E. Ichiishi, A. Harmalkar, J.J. Gray, A.M.J.J. Bonvin, F. Ambrosetti, R.V. Honorato, Z. Jandova, B. Jiménez-García, P.I. Koukos, S. Van Keulen, C.W. Van Noort, M. Réau, J. Roel-Touris, S. Kotelnikov, D. Padhorny, K.A. Porter, A. Alekseenko, M. Ignatov, I. Desta, R. Ashizawa, Z. Sun, U. Ghani, N. Hashemi, S. Vajda, D. Kozakov, M. Rosell, L.A. Rodrguez-Lumbreras, J. Fernandez-Recio, A. Karczynska, S. Grudinin, Y. Yan, H. Li, P. Lin, S.-Y. Huang, C. Christoffer, G. Terashi, J. Verburgt, D. Sarkar, T. Aderinwale, X. Wang, D. Kihara, T. Nakamura, Y. Hanazono, R. Gowthaman, J. D Guest, R. Yin, G. Taherzadeh, B.G. Pierce, D. Barradas-Bautista, Z. Cao, L. Cavallo, R. Oliva, Y. Sun, S. Zhu, Y. Shen, T. Park, H. Woo, J. Yang, S. Kwon, J. Won, C. Seok, Y. Kiyota, S. Kobayashi, Y. Harada, M. Takeda-Shitaka, P.J. Kundrotas, A. Singh, I.A. Vakser, J. Dapkūnas, K. Olechnovič, Č. Venclovas, R. Duan, L. Qiu, S. Zhang, X. Zou, S.J. Wodak. Prediction of protein assemblies, the next frontier: The CASP14-CAPRI experiment. *Proteins: Struct. Func. Bioinf.*, **2021**, 80, 1800-1823.

263. M. Kogut, Z. Gong, C. Tang, **A. Liwo**. Pseudopotentials for coarse-grained cross-link-assisted modeling of protein structures. *J. Comput. Chem.*, **2021**, 42, 2054–2067.

262. F. Gondelaud, M. Bouaki, A. Le Fèvre, A.E. Miele, F. Chirot, B. Duclos, **A. Liwo**, S. Ricard-Blum. Extended disorder at the cell surface: the conformational landscape of the ectodomains of syndecans. *Matrix Biol. Plus*, **2021**, **12**, 100081.

261. A. Antoniak, I. Biskupek, K.K. Bojarski, C. Czaplewski, A. Giełdoń, M. Kogut, M.M. Kogut, P. Krupa, A.G. Lipska, **A. Liwo**, E.A. Lubecka, M. Marcisz, M. Maszota-Zieleniak, S.A. Samsonov, A.K. Sieradzan, M.J. Ślusarz, R. Ślusarz, P.A. Wesołowski, K. Zięba. Modeling protein structures with the coarse-grained UNRES force field in the CASP14 experiment. *J. Mol. Graph. Model.*, **2021**, 108, 108008.

260. E.A. Lubecka, **A. Liwo**. ESCASA: Analutical estimation of atomic coordinates from coarse-grained geometry for nuclear-magnetic-resonance-assisted protein structure modeling. I. Backbone and H^{β} protons. *J. Comput. Chem.*, **2021**, 42, 1579-1589.

259. P. Krupa, A.S. Karczyńska, M.A. Mozolewska, **A. Liwo**, C. Czaplewski. UNRES-Dock – protein-protein and peptide-protein docking by coarse-grained replica-exchange MD simulations. *Bioinformatics*, **2021**, 37, 1613-1615.

258. **A. Liwo**, C. Czaplewski, A.K. Sieradzan, E.A. Lubecka, A.G. Lipska, Ł. Golon, A. Karczyńska, P. Krupa, M.A. Mozolewska, M. Makowski, R. Ganzynkowicz, A. Giełdoń, M. Maciejczyk. Scale-consistent approach ro the derivation of coarse-grained force fields for simulating structure, dynamics, and thermodynamics of biopolymers. *Prog. Mol. Biol. Trans. Sci.*, **2020**, 170, 73-121.

257. G.J.A. Sevink, **J.A. Liwo**, P. Asinari, D. MacKernan, G. Milano, I. Pagonabarraga. Unfolding the prospects of computational (bio)materials modeling. *J. Chem. Phys.*, **2020**, 100901.

256. K. Zięba, C. Czaplewski, **A. Liwo**, G. Graziano. Hydrophobic hydration and pairwise hydrophobic interaction of Lennard-Jones and Mie particles in different water models. *Phys. Chem. Chem. Phys.*, **2020**, 2020, 22, 4758.

255. A. Karczyńska, K. Zięba, U. Uciechowska, M.A. Mozolewska, P. Krupa, E.A. Lubecka, A.G. Lipska, C. Sikorska, S.A. Samsonov, A.K. Sieradzan, A. Giełdoń, **A. Liwo**, R. Ślusarz, M. Ślusarz, J. Lee, K. Joo, C. Czaplewski. Improved Consensus-Fragment Selection in Template-Assisted Prediction of Protein Structures with the UNRES Force Field in CASP13. *J. Chem. Inf. Model.*, **2020**, 60, 1844-1864..

254. **A. Liwo**, C. Czaplewski. Extension of the force-matching method to coarse-grained models with axially-symmetric sites to produce transferable force fields: application to the UNRES model of proteins. *J. Chem. Phys.*, **2020**, 152, 054902.

253. M.F. Lensink, G. Brysbaert, N.N. Sameer, V.R.A.G. Chaleil, T. Gerguri, P.A. Bates, E.L.A. Carbone, S. Grudinin, R. Kong, R.-R. Liu, X.-M. Xu, H. Shi, S. Chang, M. Eisenstein, A. Karczynska, C. Czaplewski, E. Lubecka, A. Lipska, P. Krupa, M. Mozolewska, Ł. Golon, S. Samsonov, **A. Liwo**, S. Crivelli, G. Pagès, M. Karasikov, M. Kadukova, Y. Yan, S.-Y. Huang, M. Rosell, L.A. Rodrguez-Lumbreras, M. Romero-Durana, L. Díaz-Bueno, J. Fernandez-Recio, C. Christoffer, G. Terashi, W.-H. Shin, T. Aderinwale, S. Raghavendra, M.V. Subraman, D. Kihara, D. Kozakov, S. Vajda, K. Porter, D. Padhorny, I. Desta, D. Beglov, M. Ignatov, S. Kotelnikov, I.H. Moal, D.W. Ritchie, I. Chauvot de Beauchêne, B. Maigret, M.-D. Devignes, M.E. Ruiz Echartea, D. Brradas-Bautista, Z. Cao, L. Cavallo, R. Oliva, Y. Cao, Y. Shen, M. Baek, T. Park, H. Woo, C. Seok, M. Braitbard, L. Bitton, D. Scheidman-Duhovny, J. Dapkunas, K. Olechnovič, Č. Venclovas, P.J. Kundrotas, S. Belkin, D. Chakravarty, V.D. Badal, I.A. Vakser, T. Vreven, S. Vangaveti, T. Borrman, Z. Weng, J.D. Guest, R. Gowthaman, B.G. Pierce, X. Xu, R. Duan, L. Qiu, J. Hou, B.R. Merideth, Z. Ma, J. Cheng, X. Zou, P.I. Koukos, J. Roel-Touris, F. Ambrosetti, C. Geng, J. Scharschmidt, M.E. Trellet, A.S.J. Melquiond, L. Xue, B. Jiménez-García, C.W. van Noort, R.V. Honorato, A.M.J.J. Bonvin, S.J. Wodak. Blind prediction of homo- and hetero-protein complexes: The CASP13-CAPRI experiment. *Proteins: Struct. Func. Bioinf.*, **2019**, 87, 1200-1221. ‘

252. J. E. Fajardo, R. Shrestha, N. Gil, A. Belsom, S. N. Crivelli, C. Czaplewski, K. Fidelis, S. Grudinin, M. Karasikov, A. S. Karczyńska, A. Kryshtafovych, A. Leitner, **A. Liwo**, E. A. Lubecka, B. Monastyrskyy, G. Pagès, J. Rappsilber, A. K. Sieradzan, C. Sikorska, E. Trabjerg, A. Fiser. Assessment of chemical-crosslink-assisted protein structure modeling in CASP13. *Proteins*, **2019**, 87, 1283-1297.

251. G. Kohut, A. Sieradzan, F. Zsila, T. Júhász, S. Bősze, A. Liwo, S. A. Samsonov, T. Beke-Somfai. The molecular mechanism of structural changes in the antimicrobial peptide CM15 upon a complex formation with drug molecule suramin: a computational analysis. *Phys. Chem. Chem. Phys.*, **2019**, 21, 10644.

250. J. Potthoff, K. K. Bojarski, G. Kohut, A. G. Lipska, **A. Liwo**, E. Kessler, S. Ricard-Blum, S. A. Samsonov. Analysis of procollagen C-proteinase enhancer-1/glycosaminoglycan binding sites and of the potential role of calcium ions in the interaction. *Int. J. Mol. Sci.*, **2019**, 20, 5021; doi:10.3390/ijms20205021

249. K. Zięba, M. Ślusarz, R. Ślusarz, **A. Liwo**, C. Czaplewski, A. K. Sieradzan. Extension of the UNRES coarse-grained force field to membrane proteins in the lipid bilayer. *J. Phys. Chem. B*, **2019**, 123, 7829-7839

248. E. A. Lubecka, A. S. Karczyńska, A. G. Lipska, A. K. Sieradzan, K. Zięba, C. Sikorska, U. Uciechowska, S. A. Samsonov, P. Krupa, M. A. Mozolewska, Ł. Golon, A. Giełdoń, C. Czaplewski, R. Ślusarz, M. Ślusarz, S. N. Crivelli, **A. Liwo**. Evaluation of the scale-consistent UNRES force field in template-free prediction of protein structures in the CASP13 experiment. *J. Molec. Graphics Modeling*, **2019**, 92, 154-166.

247. A. K. Sieradzan, M. Bogunia, P. Mech, R. Ganzynkowicz, A. Giedoń, **A. Liwo**, M. Makowski. Introduction of phosphorylated residues into the UNRES coarse-grained model: toward modeling of signaling processes. *J. Phys. Chem. B*, **2019**, 119, 8526–8534.

246. E. Lubecka, **A. Liwo**. Introduction of a bounded penalty function in contact-assisted simulations of protein structures to omit false restraints. *J. Comput. Chem.*, **2019**, 40, 2164–2178.

245. S. A. Samsonov, E. A. Lubecka, K. K. Bojarski, R. Ganzynkowicz, **A. Liwo**. Local and long range potentials for heparin-protein systems for coarse-grained simulations. *Biopolymers*. **2019**, 110, e23269.

244. **A. Liwo**, A. K. Sieradzan, A. G. Lipska, C. Czaplewski, I. Joung, W. Żmudziska, A. Hałabis, S. Ołdziej. A general method for the derivation of the functional forms of the effective energy terms in coarse-grained energy functions of polymers. III. Determination of scale-consistent backbone-local and correlation potentials in the UNRES force field and force-field calibration and validation. *J. Chem. Phys.*, **2019**, 150, 155104.

243. E. Faraggi, P. Krupa, M.A. Mozolewska, **A. Liwo**, A. Kloczkowski. Reoptimized UNRES potential for protein model quality assessment. *Genes*, **2018**, 9, 601.

242. A.K. Sieradzan, A. Giełdoń, Y. Yin, Y. He, H.A. Scheraga, **A. Liwo**. A new protein nucleic-acid coarse-grained force field based on the UNRES and NARES-2P force fields. *J. Comput. Chem.*, **2018**, 29, 2345-2349.

241. G. Kohut, **A. Liwo**, S. Bősze, T. Beke-Somfai, S.A. Samsonov. Protein-Ligand Interaction Energy-Based Entropy Calculations: Fundamental Challenges For Flexible Systems. *J. Phys. Chem. B*, **2018**, 122, 7821–7827.

240. A.K. Sieradzan, Ł. Golon, **A. Liwo**. Prediction of DNA and RNA structure with the NARES-2P force field and conformational space annealing. *Phys. Chem. Chem. Phys.*, **2018**, 20, 19656–19663.

239. S.D. Vallet, A.E. Miele, U. Uciechowska-Kaczmarzyk, **A. Liwo**, B. Duclos, S.A. Samsonov, S. Ricard-Blum. Insights into the structure and dynamics of lysyl oxidase propeptide, a flexible protein with numerous partners. *Sci. Rep*, **2018**, 8, 11768.

238. C. Keasar, L.J. McGuffin, E.B. Wallner, G. Chopra, B. Adhikari, D. Bhattacharya, L. Blake, L.O. Bortot, R.Z. Cao, B.K. Dhanasekaran, I. Dimas, R.A. Faccioli, E. Faraggi, R. Ganzynkowicz, S. Ghosh, S. Ghosh, A. Giełdoń, Ł. Golon, Y. He, L. Heo, J. Hou, J M. Khan, F. Khatib, G.A. Khoury, C. Kieslich, D.E. Kim, P. Krupa, G.R. Lee, H.B. Li, J.L. Li, A.

Lipska, **A. Liwo**, A.H.A. Maghrabi, A. Hassan, M. Mirdita, S. Mirzaei, M.A. Mozolewska, M. Onel, S. Ovchinnikov, A. Shah, U. Shah, T. Sidi, A.K. Sieradzan, M. Ślusarz, R. Ślusarz, J. Smadbeck, P. Tamamis, T.N. Phanourios, T. Wirecki, Y.P. Yin, Y. Zhang, J. Bacardit, M. Baranowski, N. Chapman, S. Cooper, A. Defelicibus, J. Flatten, B. Koepnick, Z. Popovic, B. Zaborowski, D. Baker, J.L. Cheng, C. Czaplewski, A.C.B. Delbem, A. Claudio, C. Floudas, A. Kloczkowski, S. Ołdziej, M. Levitt, H.A. Scheraga, C. Seok, J. Söding, S. Vishveshwara, D. Xu, S.N. Crivelli, Foldit Players. An analysis and evaluation of the WeFold collaborative for protein structure prediction and its pipelines in CASP11 and CASP12. *Sci. Rep.*, **2018**, 8, 9939.

237. A. Karczyńska, M.A. Mozolewska, P. Krupa, A. Giełdoń, K.K. Bojarski, B. Zaborowski, **A. Liwo**, R. Ślusarz, M. Ślusarz, J. Lee, K. Joo, Cezary Czaplewski. Use of the UNRES force field in template-based prediction of protein structures and the refinement of server models: Test with CASP12 targets. *J. Molec. Graphics Modeling*, **2018**, 83, 92–99.

236. C. Czaplewski, A. Karczyńska, A.K. Sieradzan, **A. Liwo**. UNRES server for physics-based coarse-grained simulations and prediction of protein structure, dynamics and thermodynamics. *Nucleic Acids Research*, **2018**, 46, W304-W309.

235. M.J. Grzeszczuk, A. Bąk, A.M. Banaś, P. Urbanowicz, S. Dunin-Horkawicz, A. Giełdoń, C. Czaplewski, **A. Liwo**, E.K. Jagusztyn-Krynicka. Impact of selected amino acids of HP0377 (Helicobacter pylori thiol oxidoreductase) on its functioning as a CcmG (cytochrome c maturation) protein and Dsb (disulfide bond) isomerase. *PLoS ONE*, **2018**, 13(4): e0195358.

234. A.S. Karczyńska, M.A. Mozolewska, P. Krupa, A. Giełdoń, **A. Liwo**, C. Czaplewski. Prediction of protein structure with the coarse-grained UNRES force field assisted by small X-ray scattering data and knowledge-based information. *Proteins: Struct. Func. Bioinfo.*, **2018**, 86 (S1), 228-239.

233. A.S. Karczyńska, C. Czaplewski, P. Krupa, M.A. Mozolewska, K. Joo, J. Lee, **A. Liwo**. Ergodicity and Model Quality in Template-Restrained Canonical and Temperature/Hamiltonian Replica Exchange Coarse-Grained Molecular Dynamics Simulations of Proteins *J. Comput. Chem.*,**2017**, 38, 2730–2746.

232. E.A. Lubecka, **A. Liwo**. A general method for the derivation of the functional forms of the effective energy terms in coarse-grained energy functions of polymers. II. Backbone-local potentials of coarse-grained O1→4-bonded polyglucose chains. J. Chem. Phys. **2017**, 146, 124106.

231. P. Krupa, A. Hałabis, W. Żmudzińska, S. Ołdziej, H.A. Scheraga, **A. Liwo**. Maximum Likelihood Calibration of the UNRES Force Field for Simulation of Protein Structure and Dynamics. *J. Chem. Inf. Model.* **2017**, 57, 2364-2377

230. P. Krupa, A.K. Sieradzan, M.A. Mozolewska, H. Li, **A. Liwo**, H.A. Scheraga. Dynamics of Disulfide-Bond Disruption and Formation in the Thermal Unfolding of Ribonuclease A. *J. Chem. Theory Comput.*, **2017**, 13, 5721-5730.

229. M.A. Mozolewska, A.K. Sieradzan, A. Niadzvedstki, C. Czaplewski, **A. Liwo**, P. Krupa. Role of the sulfur to α-carbon thioether bridges in thurincin H. *J. Biomol. Struct. Dyn.*, **2017**, 35, 2868-2879.

228. A.K. Sieradzan, M. Makowski, A. Augustynowicz, **A. Liwo**. A general method for the derivation of the functional forms of the effective energy terms in coarse-grained energy functions of polymers. I. Backbone potentials of coarse-grained polypeptide chains. *J. Chem. Phys.*, **2017**, 146, 124106.

227. T. Johnston, B. Zhang, **A. Liwo**, S. Crivelli, M. Taufer. *In situ* data analytics and indexing of protein trajectories. *J. Comput. Chem.*, **2017**, 38, 1419-1430.

226. M. Makowski, **A. Liwo**, H.A. Scheraga. Simple physics-based analytical formulas for the potentials of mean force of the interaction of amino acid side chains in water. VII. Charged-hydrophobic/polar and polar-hydrophobic/polar side chains. *J. Phys. Chem. B*, **2017**, 121, 379-390.

225. M.A. Mozolewska, P. Krupa, B. Zaborowski, **A. Liwo**, J. Lee, K. Joo, C. Czaplewski. Use of Restraints from Consensus Fragments of Multiple Server Models to Enhance Protein-Structure Prediction Capability of the UNRES Force Field. *J. Chem. Inf. Model.*, **2016**, 56, 2263–2279.

224. P. Krupa, M.A. Mozolewska, M. Wiśniewska, Y. Yin, Y. He, A.K. Sieradzan, R. Ganzynkowicz, A.G. Lipska, A. Karczyńska, M. Ślusarz, R. Ślusarz, A. Giełdoń, C. Czaplewski, D. Jagieła, B. Zaborowski, H.A. Scheraga, **A. Liwo**. Performance of protein-structure predictions with the physics-based UNRES force field in CASP11. *Bioinformatics*, **2016**, 32, 3270-3278.

223. A.G. Lipska, S.R. Seidman, A.K. Sieradzan, A. Giełdoń, **A. Liwo**, H.A. Scheraga. Molecular dynamics of protein A and a WW domain with a united-residue model including hydrodynamic interaction. *J. Chem. Phys.*, **2016**, 144, 184110.

222. Y. He, **A. Liwo**, H.A. Scheraga. Optimization of a Nucleic Acids united-RESidue 2-Point model (NARES-2P) with a maximum-likelihood approach. *J. Chem. Phys.*, **2015**, 143, 243111.

221. B. Zaborowski, D. Jagieła, C. Czaplewski, A. Hałabis, A. Lewandowska, W. Żmudzińska, S. Ołdziej, A. Karczyńska, C. Omieczynski, T. Wirecki, **A. Liwo**. A maximum-likelihood approach to force-field calibration. *J. Chem. Inf. Model.*, **2015**, 55, 2050–2070.

220. M.A. Mozolewska, P. Krupa, H.A. Scheraga, **A. Liwo**. Molecular modeling of the binding modes of the iron-sulfur protein to the Jac1 co-chaperone from Saccharomyces cerevisiae by all-atom and coarse-grained approaches. *Proteins: Struct. Funct. Bioinfo.*, **2015**, 83, 1414–1426.

219. Y. Yin, A.K. Sieradzan, **A. Liwo**, Y. He, H.A. Scheraga. Physics-based Potentials for coarse-grained modeling of protein DNA interactions. *J. Chem. Theory Comput.*, **2015**, 11, 1792–1808.

218. P. Krupa, M.A. Mozolewska, K. Joo, J. Lee, C. Czaplewski, **A. Liwo**. Prediction of protein structure by template-based modeling combined with the UNRES force field. *J. Chem. Inf. Model.*, **2015**, 55, 1271–1281.

217. A.K. Sieradzan, P. Krupa, H.A. Scheraga, **A. Liwo**, C. Czaplewski. Physics-based potentials for the coupling between backbone- and side-chain-local conformational states in the united residue (UNRES) force field for protein simulations. *J. Chem. Theory Comput.*, **2015**, 11, 817-831.

216. A.G. Lipska, A.K. Sieradzan, P. Krupa, M. Mozolewska, S. D'Auria, **A. Liwo**. Studies of conformational changes of an arginine-binding protein from Thermotoga maritima in the presence and absence of ligand via molecular dynamics simulations with the coarse-grained UNRES force field. *J. Molec. Modeling*, **2015**, 21,10.1007/s00894-015-2609-1

215. E.I. Gołaś, C. Czaplewski, H.A. Scheraga, **A. Liwo**. Common functionally important motions of the nucleotide-binding domain of Hsp70. *Proteins: Struct. Func. Bioinf.*, **2015**, 83, 282-299.

214. M. Wiśniewska, E. Sobolewski, S. Ołdziej, A. Liwo, H.A. Scheraga, M. Makowski. Theoretical studies of interactions between O-phosphorylated and standard amino-acid side chain models in water. *J. Phys. Chem. B*, **2015**, 119, 8526-8534.

213. R. Zhou, G.G. Maisuradze, D. Suol, T. Todorovski, M.J. Macias, Y. Xiao, H.A. Scheraga, C. Czaplewski, **A. Liwo**. Folding kinetics of WW domains with the united residue force field for bridging microscopic motions and experimental measurements. *Proc. Natl. Acad. Sci. U.S.A*, **2014**, 111, 18243–18248.

212. M. Maciejczyk, A. Spasic, **A. Liwo**, H.A. Scheraga DNA Duplex Formation with a Coarse-Grained Model. J. Chem. Theory Comput., **2014**, 10, 5020-5035.

211. G.A. Khoury, **A. Liwo**, F. Khatib, H. Zhou, G. Chopra, J. Bacardit, L.O. Bortot, R.A. Faccioli, X. Deng, Y. He, P. Krupa, J. Li, M.A. Mozolewska, A.K. Sieradzan, J. Smadbeck, T. Wirecki, S. Cooper, J. Flatten, K. Xu, D. Baker, J. Cheng, A.C.B. Delbem, C.A. Floudas, C. Keasar, M. Levitt, Z. Popovič, H.A. Scheraga, J. Skolnick, S.N. Crivelli, and Foldit Players. WeFold: A coopetition for protein structure prediction. *Proteins: Struct. Funct. Bioinfo.*, **2014**, 82, 1850-1868.

210. **A. Liwo**, M. Baranowski, C. Czaplewski, E. Gołaś, Y. He, D. Jagieła, P. Krupa, M. Maciejczyk, M. Makowski, M.A Mozolewska, A. Niadzvedtski, S. Ołdziej, H.A. Scheraga, A.K. Sieradzan, R. Ślusarz, T. Wirecki, Y. Yin, B. Zaborowski. A unified coarse-grained model of biological macromolecules based on mean-field multipole.multipole interactions. *J. Molec. Model.*, **2014**, 20, 1-15.

209. K. Kachlishvili, G.G. Maisuradze, O.A. Martin, **A. Liwo**, J.A. Vila, H.A. Scheraga. Accounting for a mirror-image conformation as a subtle effect in protein folding. *Proc. Natl. Acad. Sci. USA*, **2014**, 111, 8458-8463.

208. A. K. Sieradzan, A. Niadzvedtski, H.A. Scheraga, **A. Liwo**, Revised backbone-virtual-bond-angle potentials to treat the L- and D-amino acid residues in the coarse-grained united residue (UNRES) force field. *J. Chem. Theory Comput.*, **2014**, 10, 2194-2203.

207. A. Krokhotin, **A. Liwo**, G.G. Maisuradze, A.J. Niemi, H.A. Scheraga. Kinks, loops, and protein folding, with protein A as an example. J. Chem. Phys., **2014**, 140, 025101.

206. P. Krupa, A.K. Sieradzan, S. Rackovsky, M. Baranowski, S. Ołdziej, H.A. Scheraga, **A. Liwo**, C. Czaplewski. Improvement of the treatment of loop structures in the UNRES force field by inclusion of coupling between backbone- and side-chain-local conformational states *J. Chem. Theory Comput.*, **2013**, 4620-4632.

205. Y. He, M.A. Mozolewska, P. Krupa, A.K. Sieradzan, T.K. Wirecki, **A. Liwo**, K. Kachlishvili, S. Rackovsky, D. Jagieła, R. Ślusarz, C.R. Czaplewski, S. Ołdziej, H.A. Scheraga, Lessons from application of the UNRES force field to predictions of structures of CASP10 targets. *Proc. Natl. Acad. Sci. U.S.A.*, **2013**, 110, 14936-14941.

204. G. Maisuradze, **A. Liwo**, P. Senet, H.A. Scheraga. Local vs global motions in protein folding, *J. Chem. Theory Comput.*, **2013**, 9, 2907-2921.

203. **A. Liwo**. Coarse graining: a tool for large-scale simulations or more? *Phys. Scr.*, **2013**, 87, 058502.

202. Y. He, M. Maciejczyk, S. Ołdziej, H.A. Scheraga, **A. Liwo**. Mean-field interactions between nucleic-acid-base dipoles can drive the formation of a double helix, *Phys. Rev. Lett.*, **2013**, 110, 098101.

201. M. Makowska, **A. Liwo**, L. Chmurzyński, H.A. Scheraga, Influence of the length of the alanine spacer on the acidic-basic properties of the Ac-Lys-$(Ala)_n$-Lys-NH_2 peptides (n=0, 1, 2, ..., 5), *J. Sol. Chem.*, **2012**, 41, 1738-1746.

200. D. Lapidus, V. Duka, V. Stonkus, C. Czaplewski, **A. Liwo**, S. Ventura, I. Liepina. Multiple β-sheet molecular dynamics of amyloid formation from two Abl-SH3 domain peptides. *Biopolymers: Peptide Science*, **2012**, 86, 557–566.

199. A.K. Sieradzan, U.H.E. Hansmann, H.A. Scheraga, **A. Liwo**. Extension of UNRES force field to treat polypeptide chains with D-amino-acid residues. *J. Chem. Theory Comput.*, **2012**, 8, 4746–4757.

198. A. Krokhotin, **A. Liwo**, A.J. Niemi, H.A. Scheraga. Coexistence of phases in a protein heterodimer. *J. Chem. Phys.*, **2012**, 137, 035101.

197. A.K. Sieradzan, **A. Liwo**, U.H.E. Hansmann. Folding and self-assembly of a small protein complex. *J. Chem. Theory Comput.*, **2012**, 8, 3416–3422.

196. G.G. Maisuradze, R. Zhou, **A. Liwo**, Y. Xiao, H.A. Scheraga. Effects of mutation, truncation, and temperature on the folding kinetics of a WW domain. *J. Mol. Biol.*, **2012**, 420, 350–365.

195. A. Hałabis, W. Żmudzińska, **A. Liwo**, S. Ołdziej. Conformational dynamics of the Trp-Cage miniprotein at its folding temperature. *J. Phys. Chem. B*, **2012**, 23, 6898–6907.

194. E. Sobolewski, S. Ołdziej, M. Wiśniewska, **A. Liwo**, M. Makowski. Toward temperature-dependent coarse-grained potentials of side-chain interactions for protein folding simulations. II. Molecular dynamics study of pairs of different types of interactions in water at various temperatures *J. Phys. Chem. B*, **2012**, 23, 6844-6853.

193. E. Golas, G.G. Maisuradze, P. Senet, S. Ołdziej, C. Czaplewski, H. A. Scheraga, **A. Liwo**. Simulation of the opening and closing of Hsp70 chaperones by coarse-grained molecular dynamics. *J. Chem. Theor. Comput.*, **2012**, 8, 1750–1764.

192. A.K. Sieradzan, H.A. Scheraga, **A. Liwo**. Determination of effective potentials for the stretching of $C^{\alpha} \cdots C^{\alpha}$ virtual bonds in polypeptide chains for coarse-grained simulations of proteins from ab initio energy surfaces of N-Methylacetamide and N-Acetylpyrrolidine. *J. Chem. Theor. Comput.*, **2012**, 8, 1334-1343.

191. Y. Yin, G.G. Maisuradze, **A. Liwo**, H.A. Scheraga. Hidden protein folding pathways in free-energy landscapes uncovered by network analysis. *J. Chem. Theory Comput.*, **2012**, 8, 1176-1189.

190. J. Makowska, **A. Liwo**, W. Żmudzińska, A. Lewandowska, L. Chmurzyński, H.A. Scheraga. Like-charged residues at the ends of oligoalanine sequences might induce a chain reversal. *Biopolymers*, **2012**, 97, 240-249.

189. A. Rojas, **A. Liwo**, H.A. Scheraga. A study of the α-helical intermediate preceding the aggregation of the amino-terminal fragment of the Aβ-amyloid peptide (1-28). *J. Phys. Chem. B*, **2011**, 115, 12978-12983.

188. M. Makowski, **A. Liwo**, H.A. Scheraga. Simple physics-based analytical formulas for the potentials of mean force of the interaction of amino-acid side chains in water. VI. Oppositely charged side chains. *J. Phys. Chem. B*, **2011**, 115, 6130-6137.

187. M. Makowski, **A. Liwo**, E. Sobolewski, H.A. Scheraga. Simple physics-based analytical formulas for the potentials of mean force of the interaction of amino-acid side chains in water. V. Like-charged side chains. *J. Phys. Chem. B*, **2011**, 115, 6119-6129.

186. Y. He, **A. Liwo**, H. Weinstein, H.A. Scheraga, PDZ Binding to the BAR Domain of PICK1 is Elucidated by Coarse-grained Molecular Dynamics. *J. Mol. Biol.*, **2011**, 405, 298-314.

185. M. Kozak, A. Lewandowska, S. Ołdziej, S. Rodziewicz-Motowidło, **A. Liwo**, Combination of SAXS and NMR techniques as a tool for the determination of peptide structure in solution. *J. Phys. Chem. Letters*, **2010**, 1, 3128-3131.

184. A. Rojas, **A. Liwo**, D. Browne, H. A. Scheraga, Mechanism of fiber assembly; treatment of Aβ-peptide peptide aggregation with a coarse-grained united-residue force field. *J. Mol. Biol.*, **2010**, 404, 537-552.

183. G.G. Maisuradze, **A. Liwo**, S. Ołdziej, H.A. Scheraga. Evidence, from simulations, of a single state with residual native structure at the thermal denaturation midpoint of a small globular protein. *J. Am. Chem. Soc*, **2010**, 132, 9444-9452.

182. M. Maciejczyk, **A. Liwo**, H.A. Scheraga. Coarse-grained model of nucleic acid bases. *J. Comput. Chem.*, **2010**, 31, 1644-1655.

181. G.G. Maisuradze, P. Senet, C. Czaplewski, **A. Liwo**, H.A. Scheraga. Investigation of protein folding by coarse-grained molecular dynamics with the UNRES force field. *J. Phys. Chem. A*, **2010**, 114, 4471-4485.

180. A. Lewandowska, S. Ołdziej, **A. Liwo**, H.A. Scheraga. Mechanism of formation of the C-terminal β-hairpin of the B3 domain of the immunoglobulin binding protein G from Streptococcus. Part IV. Implication for the mechanism of folding of the parent protein. *Biopolymers*, **2010**, 93, 469-480.

179. U. Kozłowska, G.G. Maisuradze, **A. Liwo**, H.A. Scheraga. Determination of side-chain-rotamer and side-chain and backbone virtual-bond-stretching potentials of mean force from AM1 energy surfaces of terminally-blocked amino-acid residues, for coarse-grained simulations of protein structure and folding. 2. Results, comparison with statistical potentials, and implementation in the UNRES force field. *J. Comput. Chem.*, **2010**, 31, 1154-1167.

178. U. Kozłowska, **A. Liwo**. H.A. Scheraga. Determination of side-chain-rotamer and side-chain and backbone virtual-bond-stretching potentials of mean force from AM1 energy surfaces of terminally-blocked amino-acid residues, for coarse-grained simulations of protein structure and folding. 1. The Method. *J. Comput. Chem.*, **2010**, 31, 1143-1153.

177. **A. Liwo**, S. Ołdziej, C. Czaplewski, D.S. Kleinerman, P. Blood, H.A. Scheraga. Implementation of molecular dynamics and its extensions with the coarse-grained UNRES force field on massively parallel systems; towards millisecond-scale simulations of protein structure, dynamics, and thermodynamics *J. Chem. Theor. Comput.*, **2010**, 6, 890-909.

176. G. Maisuradze, **A. Liwo**, H.A. Scheraga. Relation between free energy landscapes of proteins and dynamics. *J. Chem. Theor. Comput.*, **2010**, 6, 583-595.

175. M. Makowski, C. Czaplewski, **A. Liwo**, H.A. Scheraga. Potential of mean force of association of large hydrophobic particles: toward the nanoscale limit. *J. Phys. Chem. B*, **2010**, 114, 993-1003.

174. A. Lewandowska, S. Ołdziej, **A. Liwo**, H.A. Scheraga. Mechansm of formation of the C-terminal β-hairpin of the B3 domain of the immunoglobulin binding protein G from Streptococcus. Part III. Dynamics of long-range hydrophobic interactions. *Proteins: Struct. Funct. and Bioinf.*, **2010**, 78, 723-737.

173. E. Sobolewski, M. Makowski, S. Ołdziej, C. Czaplewski, **A. Liwo**, H.A. Scheraga. Towards temperature-dependent coarse-grained potentials of side-chain interactions for protein folding simulations. I. Molecular dynamics study of a pair of methane molecules in water at various temperatures. *PEDS*, **2009**, 22, 547-552.

172. Y. He, Y. Xiao, **A. Liwo**, H.A. Scheraga. Exploring the parameter space of the coarse-grained UNRES force field by random search: selecting a transferable medium-resolution force field. *J. Comput. Chem.*, **2009**, 30, 2127-2135.

171. G.G. Maisuradze, **A. Liwo**, H.A. Scheraga. How adequate are one- and two-dimensional free energy landscapes for protein folding dynamics? *Phys. Rev. Lett.*, **2009**, 102, 238102.

170. H. Shen, **A. Liwo**, H.A. Scherega. An improved functional form for the temperature scaling factors of the components of the mesoscopic UNRES force field for simulations of protein structure and dynamics. *J. Phys. Chem. B*, **2009**, 113, 8738-8744.

169. A. Skwierawska, W. Żmudzińska, S. Ołdziej, **A. Liwo**, H.A. Scheraga. Mechanism of formation of the C-terminal β-hairpin of the B3 domain of the immunoglobulin binding protein G from Streptococcus. II. Interplay of local backbone conformational dynamics and long-range hydrophobic interactions in hairpin formation. *Proteins: Strut. Funct. Bioinfo.*, **2009**, 76, 637-654.

168. A. Skwierawska, J. Makowska, S. Ołdziej, **A. Liwo**, H.A. Scheraga. Mechanism of formation of the C-terminal β-hairpin of the B3 domain of the immunoglobulin binding protein G from Streptococcus. I. Importance of hydrophobic interactions in stabilization of β-hairpin structure. *Proteins: Strut. Funct. Bioinfo.*, **2009**, 75, 931-953.

167. G.G. Maisuradze, **A. Liwo**, H.A. Scheraga. Principal component analysis for protein folding dynamics. *J. Mol. Biol.*, **2009**, 385, 312-329.

166. C. Czaplewski, S. Kalinowski, **A. Liwo**, H.A. Scheraga. Application of multiplexed replica exchange molecular dynamics to the UNRES force field: tests with α and $\alpha+\beta$ proteins. *J. Chem. Theor. Comput.*, **2009**, 5, 627-640.

165. S. Rodziewicz-Motowidło, J. Iwaszkiewicz, R. Sosnowska, P. Czaplewska, E. Sobolewski, A. Szymańska, K. Stachowiak, **A. Liwo**. The role of the Val57 amino-acid residue in the hinge loop of the human cystatin C. Conformational studies of the β2-L1-β3 segments of wild type human cystatin C and its mutants. *Biopolymers*, **2009**, 91, 373-383.

164. A. Skwierawska, S. Rodziewicz-Motowidło, S. Ołdziej, **A. Liwo**, H.A. Scheraga. Conformational studies of the α-helical 28-43 fragment of the B3 domain of the immunoglobulin binding protein G from Streptococcus. *Biopolymers: Peptide Science*, **2009**, 91, 37-51.

163. H. Shen, C. Czaplewski, **A. Liwo**, H.A. Scheraga. Implementation of a Serial Replica Exchange Method in a Physics-Based United-Residue (UNRES) Force Field. *J. Chem. Theory and Comput.*, **2008**, 4, 1386-1400.

162. M. Makowski, E. Sobolewski, C. Czaplewski, S. Ołdziej, **A. Liwo**, H.A. Scheraga. Simple physics-based analytical formulas for the potentials of mean force for the interaction of amino acid side chains in water. IV. Pairs of different hydrophobic side chains. *J. Phys. Chem. B*, **2008**, 112, 11385-11395.

161. J. Makowska, K. Bagińska, A. Skwierawska, **A. Liwo**, L. Chmurzyński, H.A. Scheraga. Influence of charge and size of terminal amino-acid residues on local conformational states and shape of alanine-based peptides. *Biopolymers: Peptide Science*, **2008**, 90, 724-732.

160. J. Makowska, K. Bagińska, **A. Liwo**, L. Chmurzyński, H.A. Scheraga. Acidic-basic properties of three alanine-based peptides containing acidic and basic side chains: Comparison between theory and experiment. *Biopolymers: Peptide Science*, **2008**, 90, 724-732.

159. D.S. Kleinerman, C. Czaplewski, **A. Liwo**, H.A. Scheraga. Implementations of Nosé-Hoover and Nosé-Poincaré termostats in mesoscopic dynamic simulations with the united-residue model of a polypeptide chain. *J. Chem. Phys.*, **2008**, 128, 245103.

158. T. Ossowski, M.O.F. Goulart, F.C. de Abreu, A.E.G. Sant'Ana, D. Zarzeczańska, P.R.B. Miranda, C.D. Costa, **A. Liwo**, P. Falkowski. Determination of the pK_a values of some biologically active and inactive hydroxyquinones. *J. Braz. Chem. Soc.*, **2008**, 19, 175-183.

157. R.K. Murarka, **A. Liwo**, H.A. Scheraga. Separation of time scale and coupling in the motion governed by the coarse-grained and fine degrees of freedom in a polypeptide backbone. *J. Chem. Phys.*, **2007**, 127, 155103.

156. E. Sobolewski, M. Makowski, C. Czaplewski, **A. Liwo**, S. Ołdziej, H.A. Scheraga. Potential of mean force of hydrophobic association: Dependence on solute size. *J. Phys. Chem. B*, **2007**, 111, 10765-10774.

155. M. Chinchio, C. Czaplewski, **A. Liwo**, S. Ołdziej, H.A. Scheraga. Dynamic formation and breaking of disulfide bonds in molecular dynamics simulations with the UNRES force field. *J. Chem. Theory and Comput.*, **2007**, 3, 1236-1248.

154. U. Kozłowska, **A. Liwo**, H.A. Scheraga. Determination of virtual-bond-angle potentials of mean force for coarse-grained simulations of protein structure and folding from ab initio energy surfaces of terminally-blocked glycine, alanine, and proline. *J. Phys.: Condens. Matter*, **2007**, 19, 285203.

153. M.Y. Niv, D.R. Ripoll, J.A. Vila, **A. Liwo**, S. Vanamee, A.K. Aggarwal, H. Weinstein, H.A. Scheraga. Topology of Type II REases revisited; structural classes and the common conserved core. *Nucl. Acids Res.*, **2007**, 35, 2227-2237.

152. H. Grajek, **A. Liwo**, W. Wiczk, G. Żurkowska. Resolution of the excitation-emission spectra of FMN in rigid poly(vinyl alcohol) matrices. *J. Photochem. Photobiol. B*, **2007**, 86, 193-198.

151. J. Makowska, S. Rodziewicz-Motowidło, K. Bagińska, M. Makowski, J.A. Vila, **A. Liwo**, L. Chmurzyński, H.A. Scheraga. Further evidence for the absence of polyproline II stretch in the XAO peptide. *Biophys. J.*, **2007**, 92, 2904-2917.

150. M. Bobrowski, **A. Liwo**, K. Hirao. Theoretical study of the energetics of the reactions of triplet dioxygen with hydroquinone, semiquinone, and their protonated forms: relation to the mechanism of superoxide generation in the respiratory chain. *J. Phys. Chem. B.*, **2007**, 111, 3543-3549.

149. M. Makowski, E. Sobolewski, C. Czaplewski, **A. Liwo**, S. Ołdziej, J.H. No, H.A. Scheraga. Simple physics-based analytical formulas for the potentials of mean force for the interaction of amino acid side chains in water. 3. Calculation and parameterization of the potentials of mean force of pairs of identical hydrophobic side chains. *J. Phys. Chem. B.*, **2007**, 111, 2925-2931.

148. M. Makowski, **A. Liwo**, K. Maksimiak, J. Makowska, H.A. Scheraga. Simple physics-based analytical formulas for the potentials of mean force for the interaction of amino acid side chains in water. 2. Tests with simple spherical systems. *J. Phys. Chem. B.*, **2007**, 111, 2917-2924.

147. M. Makowski,**A. Liwo**, H.A. Scheraga. Simple physics-based analytical formulas for the potentials of mean force for the interaction of amino acid side chains in water. 1. Approximate expression for the free energy of hydrophobic association based on a Gaussian-overlap model. *J. Phys. Chem. B.*, **2007**, 111, 2910-2916.

146. A.V. Rojas, **A. Liwo**, H.A. Scheraga. Molecular dynamics with the united-residue force field: Ab Initio folding simulations of multichain proteins. *J. Phys. Chem. B.*, **2007**, 111, 293-309.

145. **A. Liwo**, M. Khalili, C. Czaplewski, S. Kalinowski, S. Ołdziej, K. Wachucik, H.A. Scheraga. Modification and optimization of the united-residue (UNRES) potential energy function for canonical simulations. I. Temperature dependence of the effective energy function and tests of the optimization method with single training proteins. *J. Phys. Chem. B*, **2007**, 111, 260-285.

144. F. Rakowski, P. Grochowski, B. Lesyng, **A. Liwo**, H. A. Scheraga. Implementation of a symplectic multiple-time-step molecular dynamics algorithm, based on the united-residue mesoscopic potential energy function. *J. Chem. Phys.*, **2006**, 125, 204107.

143. I. Liepina, S. Ventura, C. Czaplewski, **A. Liwo**. Molecular dynamics study of amyloid formation of two Abl-SH3 domain peptides. *J. Pept. Sci.*, **2006**, 12, 780-789.

142. J. Makowska, K. Baginńska, M. Makowski, A. Jagielska, **A. Liwo**, F. Kasprzykowski, L. Chmurzyński, H.A. Scheraga. Assessment of two theoretical methods to estimate potentiometric titration curves of peptides: comparison with experiment. *J. Phys. Chem. B*, **2006**, 110, 4451-4458.

141. J. Makowska, S. Rodziewicz-Motowidło, K. Bagińska, J.A. Vila, **A. Liwo**, L. Chmurzyński, H.A. Scheraga. Polyproline II conformation is one of many local conformational states and is not an overall conformation of unfolded peptides and proteins. *Proc. Natl. Acad. Sci. USA*, **2006**, 103, 1744-1749.

140. M. Khalili, **A. Liwo**, H.A. Scheraga. Kinetic studies of folding of the B-domain of staphylococcal protein A with molecular dynamics and a united-residue (UNRES) model of polypeptide chains. *J. Mol. Biol.*, **2006**, 355, 536-547.

139. C. Czaplewski, S. Kalinowski, **A. Liwo**, D.R. Ripoll, H.A. Scheraga. Reply to "Comment on 'Molecular Origin of Anticooperativity in Hydrophobic Association' " *J. Phys. Chem. B.*, **2005**, 109, 21222-21224.

138. C. Czaplewski, S. Kalinowski, **A. Liwo**, H. A. Scheraga. Comparison of two approaches to potential of mean force calculations of hydrophobic association: particle insertion and weighted histogram analysis methods. *Mol. Phys.*, **2005**, 103, 3153-3167.

137. I. Liepina, P.A. Janmey, C. Czaplewski, **A. Liwo**. Membrane initiated gelsolin amyloid formation. *Biopolymers*, **2005**, 80, 596-597.

136. M. Khalili, **A. Liwo**, A. Jagielska, H.A. Scheraga. Molecular dynamics with the united-residue model of polypeptide chains. II. Langevin and Berendsen-bath dynamics and tests on model α-helical systems. *J. Phys. Chem. B*, **2005**, 109, 13798-13810.

135. M. Khalili, **A. Liwo**, F. Rakowski, P. Grochowski, H.A. Scheraga. Molecular dynamics with the united-residue model of polypeptide chains. I. Lagrange equations of motion and tests of numerical stability in the microcanonical mode, *J. Phys. Chem. B*, **2005**, 109, 13785-13797.

134. S. Ołdziej, C. Czaplewski, **A. Liwo**, M. Chinchio, M. Nanias, J.A. Vila, M. Khalili, Y. A. Arnautova, A. Jagielska, M. Makowski, H. D. Schafroth, R. Kaźmierkiewicz, D. R. Ripoll, J. Pillardy, J.A. Saunders, Y.K. Kang, K.D. Gibson, H.A. Scheraga. Physics-based protein-structure prediction using a hierarchical protocol based on the UNRES force field: Assessment in two blind tests. *Proc. Natl. Acad. Sci. U.S.A.*, **2005**, 102, 7547-7552.

133. C. Czaplewski, **A. Liwo**, D.R. Ripoll, H.A. Scheraga. Molecular origin of anticooperativity in hydrophobic association. *J. Phys. Chem. B*, **2005**, 109, 8108-8119.

132. **A. Liwo**, M. Khalili, H.A. Scheraga. Ab initio simulations of protein-folding pathways by molecular dynamics with the united-residue model of polypeptide chains. *Proc. Natl. Acad. Sci. U.S.A.*, **2005**, 102, 2362-2367.

131. J. Makowska, M. Makowski, **A. Liwo**, L. Chmurzyński, Theoretical calculations of homoconjugation equilibrium constants in systems modeling acid base interactions in side chains of biomolecules using the potential of mean force. *J. Comput. Chem.*, **2005**, 235-242.

130. J. Makowska, K. Bagińska, F. Kasprzykowski, J.A. Vila, A. Jagielska, **A. Liwo**, L. Chmurzyński, H.A. Scheraga. Interplay of charge distribution and conformation for peptides: comparison of theory and experiment. *Biopolymers*, **2005**, 80, 214-224.

129. I. Liepiņa, P. Janmey, C. Czaplewski, **A. Liwo**. Towards gelsolin amyloid formation. *Biopolymers*, **2004**, 76, 543-548.

128. S. Ołdziej, J. Łągiewka, **A. Liwo**, C. Czaplewski, M. Chinchio, M. Nanias, H.A. Scheraga. Optimization of the UNRES force field by hierarchical design of the potential-energy landscape. 3. Use of many proteins in optimization. *J. Phys. Chem. B.*, **2004**, 108, 16950-16959.

127. S. Ołdziej, **A. Liwo**, C. Czaplewski, J. Pillardy, H.A. Scheraga. Optimization of the UNRES force field by hierarchical design of the potential-energy landscape. 2. Off-lattice tests of the method with single proteins. *J. Phys. Chem. B.*, **2004**, 108, 16934-16949.

126. **A. Liwo**, P. Arłukowicz, S. Ołdziej, C. Czaplewski, M. Makowski, H.A. Scheraga. Optimization of the UNRES force field by hierarchical design of the potential-energy landscape. 1. Tests of the approach using simple lattice protein models. *J. Phys. Chem. B.*, **2004**, 108, 16918-16933.

125. M. Khalili, J.A. Saunders, **A. Liwo**, S. Ołdziej, H.A. Scheraga. A united-residue force field for calcium-protein interactions. *Prot. Sci.*, **2004**, 13, 2725-2735.

124. J. Makowska, M. Makowski, A. Giełdoń, **A. Liwo**, L. Chmurzyński. Theoretical calculations of heteroconjugation equilibrium constants in systems moldeling acid-base interactions in side chains of biomolecules using the potential of mean force. *J. Phys. Chem. B*, **2004**, 108, 12222-12230.

123. M.O.F. Goulart, N.M.F. Lima, A. Euzebio, G. Sant'Ana, P.A.L. Ferraz, J.C.M. Cavalcanti, P. Falkowski, T. Ossowski, **A. Liwo**. Electrochemical studies of isolapachol with emphasis on oxygen interaction with its radical anions. *J. Electroanal. Chem.*, **2004**, 566, 25-29.

122. K. Guzow, R. Ganzynkowicz, A. Rzeska, J. Mrozek, M. Szabelski, J. Karolczak, **A. Liwo**, W. Wiczk. Photophysical properties of tyrosine and its simple derivatives studied by time-resolved fluorescence spectroscopy, global analysis and theoretical calculations. *J. Phys. Chem. B*, **2004**, 108, 3879-3889.

121. C. Czaplewski, S. Ołdziej, **A. Liwo**, H.A. Scheraga. Prediction of the structures of proteins with the UNRES force field, including dynamic formation and breaking of disulfide bonds. *Protein Eng. Des. Select.*, **2004**, 17, 29-36.

120. **A. Liwo**, S. Ołdziej, C. Czaplewski, U. Kozłowska, H.A. Scheraga. Parameterization of backbone-electrostatic and multibody contributions to the UNRES force field for protein-structure prediction from *ab initio* energy surfaces of model systems. *J. Phys. Chem. B*, **2004**, 108, 9421-9438.

119. C. Czaplewski, **A. Liwo**, J. Pillardy, S. Ołdziej, H.A. Scheraga. Improved Conformational Space Annealing method to treat β-structure with the UNRES force-field and to enhance scalability of parallel implementation. *Polymer*, **2004**, 45, 677-686.

118. K. Maksimiak, S. Rodziewicz-Motowidło, C. Czaplewski, **A. Liwo**, H.A. Scheraga. Molecular simulation study of the potentials of mean force for the interactions between models of like-charged as well as between charged and nonpolar amino-acid side chains in water. *J. Phys. Chem. B*, **2003**, 107, 13496-13504.

117. S. Ołdziej, U. Kozłowska, **A. Liwo**, H.A. Scheraga. Determination of the potentials of mean force for rotation about $C^{\alpha}\cdots C^{\alpha}$ virtual bonds in polypeptides from the *ab initio* energy surfaces of terminally-blocked glycine, alanine, and proline. *J. Phys. Chem. A*, **2003**, 107, 8035-8046.

116. C. Czaplewski, S. Rodziewicz-Motowidło, M. Dąbal, **A. Liwo**, D.R. Ripoll, H.A. Scheraga. Molecular simulation study of cooperativity in hydrophobic association: clusters of four hydrophobic particles. *Biophys. Chem.*, **2003**, 105, 339-359.

115. I. Liepiņa, P.A. Janmey, C. Czaplewski, **A. Liwo**. Molecular dynamics study of the influence of calcium ions on the conformation of gelsolin S2 domain. *J. Mol. Struct. THEOCHEM*, **2003**, 630, 309-313.

114. I. Liepiņa, C. Czaplewski, P. Janmey, **A. Liwo**. Molecular dynamics study of a gelsolin-derived peptide binding to a lipid bilayer containing phosphatidylinositol 4,5-bisphospate. *Biopolymers*, **2003**, 71, 49-70.

113. R. Kaźmierkiewicz, **A. Liwo**, H.A. Scheraga. Addition of side chains to a known backbone with defined side-chain centroids. *Biophys. Chem.*, **2003**, 100, 261-280.

112. M.O.F. Goulart, P. Falkowski, T. Ossowski, **A. Liwo**. Electrochemical study of oxygen interaction with lapachol and its radical anions. *Bioelectrochemistry*, **2003**, 59, 85-87.

111. M. Bobrowski, **A. Liwo**, S. Ołdziej, D. Jeziorek, T. Ossowski. *Ab initio* study of the mechanism of singlet-dioxygen addition to hydroxyaromatic compounds: Negative evidence for the involvement of peroxa and endoperoxide intermediates. *J. Comput. Chem.*, **2002**, 23, 1076-1089.

110. K. Brzozowski, A. Łęgowska, S. Rodziewicz-Motowidło, **A. Liwo**, K. Rolka. The study of conformational equilibrium of c[Gln-Trp-Phe-Gly-Leu-Met], a NK-2 tachykinin antagonist. *Pol. J. Chem.* **2002**, 76, 807-814.

109. S. Rodziewicz-Motowidło, K. Brzozowski, A. Łęgowska, **A. Liwo**, J. Silbering, M. Smoluch, K. Rolka. Conformational solution studies of neuropeptide gamma using CD and NMR spectroscopy. *J. Pept. Sci.* **2002**, 8, 211-226.

108. R. Kaźmierkiewicz, **A. Liwo**, H.A. Scheraga. Energy-based reconstruction of a protein backbone from its α-carbon trace by a Monte Carlo method. *J. Comput. Chem.*, **2002**, 23, 715-723.

107. **A. Liwo**, P. Arłukowicz, C. Czaplewski, S. Ołdziej, J. Pillardy, H.A. Scheraga. A method for optimizing potential-energy functions by a hierarchical design of the potential-energy landscape: Application to the UNRES force field. *Proc. Natl. Acad. Sci. U.S.A.*, **2002**, 99, 1937-1942.

106. C. Czaplewski, S. Rodziewicz-Motowidło, **A. Liwo**, D.R. Ripoll, R.J. Wawak, H.A. Scheraga. Comment on Ąnti-cooperativity in hydrophobic interactions: A simulation study of spatial dependence of three-body effects and beyond"[J. Chem. Phys. 115, 1414 (2001)]. *J. Chem. Phys.*, **2002**, 116, 2665-2667.

105. J. Malicka, M. Groth, C. Czaplewski, W. Wiczk, **A. Liwo**. Conformational studies of cyclic enkephalin analogues with L- or D-proline in position 3. *Biopolymers*, **2002**, 63, 217-231.

104. C. Czaplewski, D.R. Ripoll, **A. Liwo**, S. Rodziewicz-Motowidło, R.J. Wawak, H.A. Scheraga. Can cooperativity in hydrophobic association be reproduced correctly by implicit solvation models? *Int. J. Quant. Chem.*, **2002**, 88, 41-55.

103. J. Malicka, M. Groth, C. Czaplewski, J. Karolczak, **A. Liwo**, W. Wiczk. Influence of solvent and configuration of residues at position 2 and 3 on distance and mobility of pharmacophore group at position 1 and 4 in cyclic enkephalin analogues. *Biopolymers*, **2001**, 59, 180-190.

102. P. Drabik, **A. Liwo**, C. Czaplewski, J. Ciarkowski. The investigation of the effects of counterions in protein dynamics. *Protein Engineering*, **2001**, 14, 747-752.

101. S. Rodziewicz-Motowidlo, A. Lesner, A. Łęgowska, C. Czaplewski, **A. Liwo**, K. Rolka, R. Patacchini, L. Quartara. Synthesis, activity on NK-(3) tachykinin receptor and conformational solution studies of scyliorhinin II analogs modified at position 16. J. Pept. Res., **2001**, 58, 159-172.

100. J. Pillardy, C. Czaplewski, **A. Liwo**, W.J. Wedemeyer, J. Lee, D.R. Ripoll, P. Arlukowicz, S. Ołdziej, Y.A. Arnautova, H.A. Scheraga. Development of physics-based energy functions that predict medium-resolution structures for proteins of the α, β and α/β structural classes. *J. Phys. Chem. B*, **2001**, 105, 7299-7311.

99. **A. Liwo**, C. Czaplewski, J. Pillardy, H.A. Scheraga, Cumulant-based expressions for the multibody terms for the correlation between local and electrostatic interactions in the united-residue force field. *J. Chem. Phys.*, **2001**, 115, 2323-2347.

98. M. Groth, J. Malicka, S. Rodziewicz-Motowidło, C. Czaplewski, L. Klaudel, W. Wiczk, **A. Liwo**. Determination of conformational equilibrium of peptides in solution by NMR spectroscopy and theoretical conformational analysis: application to the calibration of mean-field solvation models. *Biopolymers*, **2001**, 60, 79-95.

97. J. Malicka, R. Ganzynkowicz, M. Groth, C. Czaplewski, J. Karolczak, **A. Liwo**, W. Wiczk. Fluorescence decay time distribution analysis of cyclic enkephalin analogues; Influence of solvent and Leu configuration in position 5 on conformation. *Acta Biochim. Pol.*, **2001**, 48, 95-102.

96. J. Pillardy, C. Czaplewski, **A. Liwo**, J. Lee, D.R. Ripoll, R. Kaźmierkiewicz, St. Ołdziej, W.J. Wedemeyer, K.D. Gibson, Y.A. Arnautova, J. Saunders, Y.-J. Ye, H.A. Scheraga. Recent improvements in prediction of protein structure by global optimization of a potential energy function. *Proc. Natl. Acad. Sci. USA*, **2001**, 98, 2329-2333.

95. J. Malicka, M. Groth, J. Karolczak, C. Czaplewski, **A. Liwo**, W. Wiczk, Influence of solvents and leucine configuration at position 5 on tryptophan fluorescence in cyclic enkephalin analogues. *Biopolymers*, **2001**, 58, 447-457.

94. L. Klaudel, S. Rodziewicz-Motowidło, **A. Liwo**, K. Rolka. A comparison of solution conformations of scyliorhinin I and its analogue with N-methyl-L-phenylalanine in position 7. *Pol. J. Chem.*, **2000**, 74, 1091-1099.

93. S. Rodziewicz-Motowidło, A. Łęgowska, X.F. Qi, C. Czaplewski, **A. Liwo**, P. Sowiński, W. Mozga, J. Olczak, J. Zabrocki, K. Rolka. Solution conformational study of Scyliorhinin I analogues with conformational constraints by two-dimensional NMR and theoretical conformational analysis. *J. Pept. Res.*, **2000**, 56, 132-146.

92. M. Bobrowski, **A. Liwo**, S. Ołdziej, D. Jeziorek, T. Ossowski, CAS MCSCF/CAS MCQDPT2 study of the mechanism of singlet-oxygen addition to 1,3-butadiene and benzene, *J. Am. Chem. Soc.*, **2000**, 122, 8112-8119.

91. C. Czaplewski, S. Rodziewicz-Motowidło, **A. Liwo**, D.R. Ripoll, R.J. Wawak, H.A. Scheraga, Molecular simulation study of cooperativity in hydrophobic association. *Prot. Sci.*, **2000**, 9, 1235-1245.

90. T. Ossowski, P. Pipka, **A. Liwo**, D. Jeziorek. Electrochemical and UV-spectrophotometric study of oxygen and superoxide anion radical interaction with anthraquinone derivatives and their radical anions. *Electrochim. Acta*, **2000**, 45, 3581-3587.

89. J. Lee, J. Pillardy, C. Czaplewski, Y. Arnautova, D.R. Ripoll, **A. Liwo**, K.D. Gibson, R.J. Wawak, H.A. Scheraga. Efficient parallel algorithms in global optimization of potential energy functions. *Comput. Phys. Comm.*, **2000**, **128**, 399-411.

88. J. Lee, **A. Liwo**, D.R. Ripoll, J. Pillardy, J.A. Saunders, K.D. Gibson, H.A. Scheraga. Hierarchical energy-based approach to protein-structure prediction; blind-test evaluation with CASP3 targets. *Int. J. Quant. Chem.*, **2000**, 77, 90-117.

87. M. Groth, J. Malicka, C. Czaplewski, S. Ołdziej, L. Łankiewicz, W. Wiczk, **A. Liwo**. Maximum entropy approach to the determination of solution conformation of flexible polypeptides by global conformational analysis and NMR spectroscopy – application to DNS^1-c-[D-A$_2$bu^2,Trp^4,Leu^5]enkephalin and DNS^1-c-[D-A$_2$bu^2, Trp^4, D-Leu^5]enkephalin. *J. Biomol. NMR*, **1999**, 4, 315-330.

86. J. Malicka, M. Groth, C. Czaplewski, **A. Liwo**, W. Wiczk. Fluorescence decay time distribution analysis of cyclic enkephalin analogues. Influence of the solvents and configuration of amino acids in position 2 and 3 on changes in conformation. *Acta Biochim. Pol.*, **1999**, 46, 615-629.

85. S. Rodziewicz, I. Wirkus-Romanowska, M. Ciurak, H. Miecznikowska, G. Kupryszewski, C. Czaplewski, **A. Liwo**, K. Rolka. Cyclic analogues of proline-rich protein fragments. Part II: Conformational studies using NMR spectroscopy and theoretical conformational analysis. *Pol. J. Chem.*, **1999**, 73, 1697-1710.

84. M. Makowski, **A. Liwo**, R. Wróbel, L. Chmurzyński. *Ab initio* study of the energetics of protonation and hydrogen bonding of pyridine N-Oxide and its derivatives *J. Phys. Chem. A*, **1999**, 103, 11104-11108.

83. J. Pillardy, **A. Liwo**, H.A. Scheraga. An efficient deformation-based global optimization method [self-consistent basin-to-deformed-basin mapping (SCBDBM)]; Application to Lennard-Jones atomic clusters. *J. Phys. Chem. A*, **1999**, 103, 9370-9377.

82. A. Bogdańska, L. Chmurzyński, T. Ossowski, **A. Liwo**, D. Jeziorek. Protolytic equilibria of dihydroxyanthraquinones in non-aqueous solutions. *Anal. Chim. Acta*, **1999**, 402, 339-343.

81. J. Zielińska, M. Makowski, K. Maj, **A. Liwo**, L. Chmurzyński. Acid-base and hydrogen-bonding equilibria in aliphatic amine and carboxylic acid systems in non-aqueous solutions. *Anal. Chim. Acta*, **1999**, 401, 317-321.

80. J. Pillardy, **A. Liwo**, M. Groth, H.A. Scheraga. An efficient deformation-based global optimization method for off-lattice polymer chains; self-consistent basin-to-deformed-basin mapping (SCBDBM). Application to united-residue polypeptide chains. *J. Phys. Chem. B*, **1999**, 103, 7353-7366.

79. J. Lee, **A. Liwo**, D.R. Ripoll, J. Pillardy, H.A. Scheraga. Calculation of Protein Conformation by Global Optimization of a potential energy function. *Proteins: Struct. Func. Genet.*, **1999**, Suppl. 3, 204-208.

78. **A. Liwo**, J. Lee, D.R. Ripoll, J. Pillardy, H.A. Scheraga. Protein structure prediction by global optimization of a potential energy function. *Proc. Natl. Acad. Sci. USA*, **1999**, 96, 5482-5485.

77. E. Kaczmarczyk, R. Wróbel, **A. Liwo**, L. Chmurzyński. Temperature dependence of the acid-base equilibrium constants of substituted pyridine N-oxides in acetonitrile. *J. Mol. Struct.*, **1999**, 477, 113-118.

76. J. Lee, **A. Liwo**, H.A. Scheraga. Energy-based de novo protein folding by conformational space annealing and an off-lattice united-residue force field: Application to the 10-55 fragment of staphylococcal protein A and to apo calbindin D9K. *Proc. Natl. Acad. Sci. USA*, **1999**, 96, 2025-2030.

75. **A. Liwo**, J. Pillardy, R. Kaźmierkiewicz, R.J. Wawak, M. Groth, C. Czaplewski, S. Ołdziej, H.A. Scheraga. Prediction of protein structure using a knowledge-based off-lattice united-residue force field and global optimization methods. *Theoretical Chemistry Accounts*, **1999**, 101, 16-20.

74. D.R. Ripoll, **A. Liwo**, H.A. Scheraga. New developments of the Electrostatically Driven Monte Carlo Method: test on the membrane-bound portion of melittin. *Biopolymers*, **1998**, 46, 117-126.

73. R.J. Wawak, J. Pillardy, **A. Liwo**, K.D. Gibson, H.A. Scheraga. Diffusion equation and distance scaling methods of global optimization: applications to crystal structure prediction. *J. Phys. Chem. A*, **1998**, 102, 2904-2918.

72. A. Wawrzynów, **A. Liwo**, E. Kaczmarczyk, L. Chmurzyński. Cationic heteroconjugation constants in the OHN^+ and NHO^+ systems in propylene carbonate: dependence on difference in basicity. *J. Solution Chem.*, **1998**, 27, 463-472.

71. A. Wawrzynów, **A. Liwo**, E. Kaczmarczyk, L. Chmurzyński. A potentiometric study of the $(OHO)^+$-type cationic heteroconjugation equilibria in propylene carbonate. *Journal of Molecular Structure*, **1998**, 448, 185-189.

70. J. Malicka, M. Groth, C. Czaplewski, **A. Liwo**, W. Wiczk, L. Łankiewicz. Computer modeling of the solution conformation of cyclic enkephalins, *Lett. Pept. Sci.*, **1998**, 5, 445-447.

69. X.W. Shi, A.B. Attygalle, **A. Liwo**, M.-H. Hao, J. Meinwald, H.R.W. Dharmaratne, W.M.A.P. Wanigaseker. Absolute stereochemistry of soulattrolide and its analogues. *J. Org. Chem.*, **1998**, 63, 1233-1238.

68. **A. Liwo**, D. Jeziorek, T. Ossowski, M. Groth. CASSCF/MCQDPT2 study on electron and hydrogen-atom transfer from ethene derivatives to singlet oxygen - implication for peroxidation processes, *Internet Journal of Chemistry*, **1998** 1, Article 13.

67. **A. Liwo**, R. Kaźmierkiewicz, C. Czaplewski, M. Groth, S. Ołdziej, R.J. Wawak, S. Rackovsky, M.R. Pincus, H.A. Scheraga. United-residue force field for off-lattice protein-structure simulations. III. Origin of backbone hydrogen-bonding cooperativity in united-residue potentials, *J. Comput. Chem.*, **1998**, 19, 259-276.

66. I. Liepiņa, M. Blanco, G. Duburs, **A. Liwo**. Spatial structure of dihydropyridines and similarity of dihydropyridines with some amino acids. *Molecular Engineering*, **1997**, 7, 401-427.

65. W. Wiczk, L. Łankiewicz, C. Czaplewski, S. Ołdziej, K. Stachowiak, A. Michniewicz, B. Micewicz, **A. Liwo**. The photophysics of tyrosine and its simple derivatives. *J. Fluorescence*, **1997**, 7, 257-266.

64. **A. Liwo**, D. Dyl, D. Jeziorek, M. Nowacka, T. Ossowski, W. Woźnicki. MCSCF study of singlet-oxygen addition to ethenol – a model of photooxidation reactions of unsaturated and aromatic compounds bearing hydroxy groups. *J. Comput. Chem.*, **1997**, 18, 1668-1681.

63. L. Chmurzyński, E. Kaczmarczyk, **A. Liwo**. A study of cationic heteroconjugation equilibria of substituted pyridine N-oxides in acetonitrile. *Anal. Chim. Acta*, **1997**, 338, 261-267.

62. L. Chmurzyński, **A. Liwo**, P. Barczyński. A potentiometric study of acid-base equilibria of substituted pyridine N-oxides in nitrobenzene. *Anal. Chim. Acta*, **1996**, 335, 147-153.

61. **A. Liwo**, D. Jeziorek, D. Dyl, T. Ossowski, L. Chmurzyński. Theoretical Study of the role of hydrogen bonding and proton transfer in oxygen reduction by semiquinones. *J. Mol. Struct. THEOCHEM*, **1997**, **388-389**, 445-449.

60. **A. Liwo**, M.R. Pincus, R.J. Wawak, S. Rackovsky, St. Ołdziej, H.A. Scheraga. A united-residue force field for off-lattice protein-structure simulations. II: Parameterization of local interactions and determination of the weights of energy terms by Z-score optimization. *J. Comput. Chem.*, **1997**, 18, 874-887.

59. **A. Liwo**, St. Ołdziej, M.R. Pincus, R.J. Wawak, S. Rackovsky, H.A. Scheraga. A united-residue force field for off-lattice protein-structure simulations. I: Functional forms and parameters of long-range side-chain interaction potentials from protein crystal data. *J. Comput. Chem.*, **1997**, 18, 849-873.

58. D. Jeziorek, T. Ossowski, **A. Liwo**, D. Dyl, M. Nowacka, W. Woźnicki. Theoretical and electrochemical study of the mechanism of anthraquinone-mediated one-electron reduction of oxygen: the involvement of adducts of dioxygen species to anthraquinones. *J. Chem. Soc. Perkin Transactions 2*, **1997**, 229-236.

57. **A. Liwo**, P. Skurski, St. Ołdziej, L. Łankiewicz, J. Malicka, W. Wiczk. A new approach to the resolution of the excitation-emission spectra of multicomponent systems. *Comput. Chem.*, **1997**, 21, 89-96.

56. W. Wiczk, L. Łankiewicz, C. Czaplewski, S. Ołdziej, K. Stachowiak, A. Michniewicz, **A. Liwo**. The photophysics of β-homotyrosine and its simple derivatives. *J. Photochem. Photobiol. A: Chemistry*, **1996**, 101, 171-181.

55. D.R. Ripoll, Yu. Vorobjev, **A. Liwo**, J.A. Vila, H.A. Scheraga. Coupling between folding and ionization equilibrium. Effects of pH on the conformational preferences of oligopeptides. *J. Mol. Biol.*, **1996**, 264, 770-783.

54. R.J. Wawak, K.D. Gibson, **A. Liwo**, H.A. Scheraga. Theoretical prediction of a crystal structure. *Proc. Natl. Acad. Sci. USA*, **1996**, 93, 1743-1746.

53. W. Wiczk, P. Rekowski, G. Kupryszewski, J. Łubkowski, S. Ołdziej, **A. Liwo**. Fluorescence and Monte Carlo conformational studies of the (1-15)galanin amide fragment. *Biophys. Chem.*, **1996**, 58, 303-312.

52. **A. Liwo**, A. Tempczyk, S. Ołdziej, M.D. Shenderovich, V.J. Hruby, S. Talluri, J. Ciarkowski, F. Kasprzykowski, L. Łankiewicz, Zbigniew Grzonka. Exploration of the Conformational Space of Oxytocin and Arginine-Vasopressin Using the Electrostatically-Driven Monte Carlo and Molecular Dynamics Methods. *Biopolymers*, **1996**, 38, 157-175.

51. **A. Liwo**, D. Jeziorek, T. Ossowski, D. Dyl, A. Tempczyk, J. Tarasiuk, M. Nowacka, E. Borowski, W. Woźnicki. Molecular modeling of singlet-oxygen binding to anthraquinones in relation to the peroxidating activity of antitumor anthraquinone drugs. *Acta Biochim. Pol.*, **1995**, 42, 445-456.

50. D.R. Ripoll, M.S. Pottle, K.D. Gibson, **A. Liwo**, H.A. Scheraga. Implementation of the ECEPP algorithm, the Monte Carlo Minimization method, and the Electrostatically Driven Monte Carlo method on the Kendall Square research KSR1 computer. *J. Comput. Chem.*, **1995**, 16, 1153-1163.

49. R. Kaźmierkiewicz, **A. Liwo**, B. Lammek. Theoretical conformational analysis of three vasopressin antagonists with a modified cyclohexyl ring in the first thioacid residue. *Int. J. Pept. Prot. Res.*, **1995**, 45, 451-458.

48. S. Ołdziej, J. Ciarkowski, **A. Liwo**, M.D. Shenderovich, Z. Grzonka. Conformational aspects of differences in requirements of oxytocin and vasopressin receptors. *Journal of Receptor & Signal Transduction Research*, **1995**, 15, 703-713.

47. J. Rak, P. Skurski, **A. Liwo**, J. Błażejowski. Theoretical studies of the structure, stability, ability to internal transformation and tautomerization, as well as reactivity of H_2PPH_2 and $HPPH_3$ molecules. *J. Am. Chem. Soc.*, **1995**, 117, 2638-2648.

46. D. Jeziorek, D. Dyl, **A. Liwo**, T. Ossowski, W. Woźnicki. Enthalpy of oxygen addition to anthraquinone derivatives determines their ability to mediating NADH oxidation. *Anti-Cancer Drug Design*, **1994**, 9, 435-448.

45. A. Angielski, **A. Liwo**, D. Konopinska, J. Ciarkowski. Theoretical Conformational analysis of insect neuropeptide proctolin and its selected analogues. *Bull. Pol. Chem. Soc. Chemistry*, **1994**, 42, 268-273.

44. Z. Pawlak, S. Kuna, M. Richert, E. Giersz, **A. Liwo**, L. Chmurzyński. Proton transfer and heteroconjugation of ammonium ions with N-bases in cyclohexanone, propanone, and butan-2-one. *J. Chem. Thermodynamics*, **1994**, 26, 483-492.

43. **A. Liwo**, S. Ołdziej, J. Ciarkowski, G. Kupryszewski, M.R. Pincus, R.J. Wawak, S. Rackovsky, H.A. Scheraga. Prediction of conformation of rat galanin in the presence and absence of water with the use of Monte Carlo methods and the ECEPP/3 force field. *J. Prot. Chem.*, **1994**, 13, 375-380.

42. **A. Liwo**, K.D. Gibson, H.A. Scheraga, P.W. Brandt-Rauf, R. Monaco, M.R. Pincus. Comparison of the low energy conformations of an oncogenic and a non-oncogenic p21 protein, neither of which binds GTP or GDP. *J. Prot. Chem.*, **1994**, 13, 237-251.

41. M. Shenderovich, W. Wilke, K. Kövér, N. Collins, V. Hruby, **A. Liwo**, J. Ciarkowski. Solution conformation of a potent bicyclic antagonist of oxytocin. *Pol. J. Chem.*, **1994**, 68, 921-927.

40. F. Kasprzykowski, P. Skurski, **A. Liwo**, L. Łankiewicz S. Ołdziej J. Łanoszka, W. Wiczk, Z.Grzonka. Conformational studies of oxytocin analogues. *Pol. J. Chem.*, **1994**, 68, 987-995.

39. M. Kawińska, L. Łankiewicz, P. Skurski, B. Micewicz, W. Wiczk St. Ołdziej, **A. Liwo**. Fluorescence energy transfer in a series of leucine-enkephalin analogues. *Pol. J. Chem.*, **1994**, 68, 975-985.

38. J. Ciarkowski, **A. Liwo**, S. Ołdziej, M. Shenderovich. Oxytocin antagonists' pharmacophore. *Pol. J. Chem.*, **1994**, 68, 929-938.

37. J. Ciarkowski, St. Ołdziej, **A. Liwo**. Mimicking the mechanism of aspartic proteases. Part 1. Molecular mechanics study. *Pol. J. Chem.*, **1994**, 68, 939-947.

36. **A. Liwo**, A. Tempczyk, T. Widernik, T. Klentak, J. Czermiński. A theoretical study of protonation and tautomerization of N-substituted aminoazobenzenes. *J. Chem. Soc. Perkin Trans. 2*, **1994**, 71-75.

35. M. Tarnowska, **A. Liwo**, M.D. Shenderovich, I. Liepiņa, A.A. Golbraikh, Z. Grzonka, A. Tempczyk. A molecular mechanics study of the effect of substitution in position 1 on the conformational space of the oxytocin/vasopressin ring. *J. Comput.-Aided Mol. Design*, **1993**, 7, 699-719.

34. **A. Liwo**, M.R. Pincus, R.J. Wawak, S. Rackovsky, H.A. Scheraga. Prediction of protein conformation on the basis of a search for compact structures; test on avian pancreatic polypeptide. *Protein Science*, **1993**, 2, 1715-1731.

33. **A. Liwo**, M.R. Pincus, R.J. Wawak, S. Rackovsky, H.A. Scheraga. Calculation of protein backbone geometry from α-carbon coordinates based on peptide-group dipole alignment. *Protein Science*, **1993**, 2, 1697-1714.

32. D. Jeziorek, D. Dyl, **A. Liwo**, W. Woźnicki, A. Tempczyk, E. Borowski. A theoretical study of the mechamism of oxygen binding by model anthraquinones II: Quantum mechanical studies of the energetics of oxygen binding to model anthraquinones. *Anti-Cancer Drug Design*, **1993**, 8, 223-235.

31. D. Jeziorek, D. Dyl, **A. Liwo**, W. Woźnicki, A. Tempczyk, E. Borowski. A theoretical study of the mechamism of oxygen binding by model anthraquinones I: Quantum mechanical evaluation of the oxygen-binding sites of 1,4-hydroquinone. *Anti-Cancer Drug Design*, **1992**, 7, 451-461.

30. M. Tarnowska, S. Ołdziej, **A. Liwo**, Z. Grzonka, E. Borowski. Investigation of the inhibition pathway of glucosamine synthase by N^3-(4-methoxyfumaroyl)-L-2,3-diaminopropanoic acid by semiempirical quantum mechanical and molecular mechanics methods. *Eur. Biophys. J.*, **1992**, 21, 273-280.

29. M. Tarnowska, S. Ołdziej, **A. Liwo**, P. Kania, F. Kasprzykowski, Z. Grzonka. MNDO study of the mechanism of the inhibition of cysteine proteinases by diazomethyl ketones. *Eur. Biophys. J.*, **1992**, 21, 217-222.

28. M.H. Hao, S. Rackovsky, **A. Liwo**, M.R. Pincus, H.A. Scheraga. Effects of compact volume and chain stiffness on the conformations of native proteins. *Proc. Natl. Acad. Sci. U.S.A.*, **1992**, 89, 6614-6618.

27. **A. Liwo**, M. Tarnowska, Z. Grzonka, A. Tempczyk. Modified Free-Wilson method for the analysis of biological activity data. *Comput. Chem.* **1992**, 16, 1-9.

26. A. Tempczyk, M. Tarnowska, **A. Liwo**, E. Borowski. A theoretical study of glucosamine synthase. II. Combined quantum and molecular mechanics simulation of sulfhydryl attack on the carboxyamide group. *Eur. Biophys. J.*, **1992**, 21, 137-145.

25. J. Tarasiuk, **A. Liwo**, W. Wojtkowiak, M. Dzieduszycka, A. Tempczyk, A. Garnier-Suillerot, S. Martelli, E. Borowski. Molecular determinants of singlet oxygen binding by anthraquinones in relation to their redox cycling activity. *Anti-Cancer Drug Design* **1991**, 6, 399-416.

24. L. Chmurzyński, **A. Liwo**. Acid-base and cationic homoconjugation equilibria of substituted pyridine N-oxides in acetone. *J. Chem. Soc. Faraday Trans.* **1991**, 87, 3853-3856.

23. M.D. Shenderovich, F. Kasprzykowski, **A. Liwo**, I. Sekacis, J. Saulitis, G.V. Nikiforovich. Conformational analysis of [Cpp^1,Sar^7, Arg^8]vasopressin by ^{1}H-NMR spectroscopy and molecular mechanics calculations. *Int. J. Pept. Protein Res.* **1991**, 38, 528-538.

22. L. Chmurzyński, **A. Liwo**. Simple methods for the estimation of ionization constants of substituted pyridine N-oxides in polar aprotic solvents and water. *J. Sol. Chem.* **1991** 20, 731-738.

21. **A. Liwo**, T. Widernik, T. Klentak. Influence of inorganic anions on the tautomeric equilibria of N-substituted aminoazobenzenes - the evidence for ionic association. *J. Sol. Chem.* **1991**, 20, 431-443.

20. Z. Pawlak, S. Kuna, M. Richert, E. Giersz, M. Wiśniewska, **A. Liwo**, L. Chmurzyński. Acidity constants of 19 protonated N-bases in cyclohexanone, acetone, and butan-2-one. *J. Chem. Thermodyn.* **1991**, 23, 135-140.

19. **A. Liwo**, K. Sokołowski, A. Wawrzynów, L. Chmurzyński. UV-spectroscopic studies on the influence of the traces of water on the protolytic equilibria of substituted pyridine N-oxides in aprotic solvents. *J. Sol. Chem.* **1990**, 19, 1113-1124.

18. L. Chmurzyński, **A. Liwo**, A. Wawrzynów, A. Tempczyk. CNDO/S-CI-nPDQ studies of the solvation effect on the UV-spectra of pyridine N-oxide and its complexes with proton. *Z. Naturforsch. B* **1990**, 45b, 719-720.

17. L. Chmurzyński, **A. Liwo**. A CNDO/2 study of the homoconjugation energies of 4-substituted pyridine N-oxides. *Z. Naturforsch. B* **1990**, 45b, 717-718.

16. J. Kostrowicki, **A. Liwo**. Determination of equilibrium parameters by minimization of an extended sum of squares. *Talanta* **1990**, 37, 645-650.

15. L. Chmurzyński, **A. Liwo**. Influence of the conjugation effect on the UV-spectra of 4-substituted pyridine N-oxides and their conjugated acids. *J. Mol. Struct.* **1990**, 218, 129-134.

14. L. Chmurzyński, **A. Liwo**, A. Tempczyk. Relationship between the electronic structure and acidic-basic properties of some substituted pyridine N-oxides. *Z. Naturforsch. B* **1989**, 44b, 1263-1270.

13. A. Tempczyk, M. Tarnowska, **A. Liwo**. A theoretical study of glucosamine synthase. I. Molecular mechanics calculations on substrate binding. *Eur. Biophys. J.* **1989**, 17, 201-210.

12. **A. Liwo**, A. Tempczyk, Z. Grzonka. Theoretical studies of the mechanism of the action of the neurohypophyseal hormones. I. Molecular electrostatic potential (MEP) and molecular electrostatic field (MEF) maps of some vasopressin analogues. *J. Comput.-Aided Mol. Design* **1989**, 3, 261-284.

11. **A. Liwo**, J. Ciarkowski. Conformation of dioxopiperazines - 8. The model building algorithm. *J. Mol. Struct. THEOCHEM* **1989**, 183, 331-340.

10. **A. Liwo**, A. Tempczyk, Z. Grzonka. Molecular mechanics calculations on deaminooxytocin and on deamino arginine vasopressin and its analogues. *J. Comput.-Aided Mol. Design* **1988**, 2, 281-309.

9. A. Wawrzynów, K. Sokołowski, **A. Liwo**, L. Chmurzyński. Experimental studies on the UV spectra of substituted pyridine N-oxides. *J. Mol. Struct.* **1988**, 174, 235-240.

8. J. Kostrowicki, **A. Liwo**, K. Sokołowski. A comparative study on some methods for computing of equilibrium concentrations. *Comput. Chem.* **1988**, 12, 293-299.

7. J. Kostrowicki, **A. Liwo**. A general method for the determination of the stoichiometry of unknown species in multicomponent systems from physicochemical measurements. *Comput. Chem.* **1987**, 11, 195-210.

6. A. Wawrzynów, **A. Liwo**, L. Chmurzyński, A. Tempczyk. A study on the UV spectra of pyridine N-oxide and 2,6-lutidine N-oxide 1:1 perchlorates solutions in propylene carbonate. *J. Mol. Struct.* **1986**, 143, 379-382.

5. L. Chmurzyński, **A. Liwo**, A. Wawrzynów, A. Tempczyk. Theoretical and experimental studies on the UV spectra of pyridine N-oxide perchlorates. *J. Mol. Struct.* **1986**, 143, 375-378.

4. Z. Warnke, C. Trojanowska, **A. Liwo**. Potentiometric study on the complex formation of some divalent metal ions with 2-aminoxyacids. *J. Coord. Chem.* **1985**, 14, 31-38.

3. **A. Liwo**, J. Ciarkowski. Origin of the ring-ring interaction in cyclic dipeptides incorporating an aromatic amino acid. *Tetrahedron Lett.* **1985**, 26, 1873-1876.

2. J. Kostrowicki, **A. Liwo**. DECFAM - A new computer-oriented algorithm for the determination of equilibrium constants from potentiometric and/or spectrophotometric measurements - II. *Comput. Chem.* **1984**, 8, 101-105.

1. J. Kostrowicki, **A. Liwo**. DECFAM - A new computer-oriented algorithm for the determination of equilibrium constants from potentiometric and/or spectrophotometric measurements - I. *Comput. Chem.* **1984**, 8, 91-99.

Original papers in non-ISI journals

7. E. Lubecka, A. K. Sieradzan, C. Czaplewski, P. Krupa, **A. Liwo**. High performance computing with coarse grained model of biological macromolecules. *Supercomputing Frontiers and Innovations*, **2018**, 5, 63-67.

6. M.A. Mozolewska, P. Krupa, B. Rasulev, **A. Liwo**, L. Leszczynski. Preliminary studies of interactions between nanotubes and toll-like receptors. *TASK Quart.*, 2014, 18, 351-455.

5. V. Duka, I. Bestel, C. Czaplewski, **A. Liwo**, I. Liepina, Molecular modeling of single β-sheet and the β-sheet stack of amyloid β-protein 25 – 35. Molecular dynamics of amylin amyloid single β-sheet. *Scientific Journal of Riga Technical University*, **2011**, 23, 62–72.

4. D. Lapidus, S. Ventura, C. Czaplewski, **A. Liwo**, I. Liepina, Molecular dynamics of amylin amyloid single β-sheet. *Scientific Journal of Riga Technical University*, **2011**, 23, 49–55.

3. R. Ganzynkowicz, **A. Liwo**, W. Wiczk. A fluorescence, ^{1}H NMR spectroscopy and molecular dynamics study of the influence of rotamer population on fluorescence decay of tyrosine, phenylalanine and their derivatives. *TASK Quart.*, **2001**, 5, 311-316.

2. D.R. Ripoll, **A. Liwo**, C. Czaplewski. The ECEPP package for conformational analysis of polypeptides. *TASK Quart.*, **1999**, 3, 313-331.

1. P. Arłukowicz, E. Arłukowicz, J. Kira, **A. Liwo**. A user-friendly interface to computer programs for the determination of the characteristics of equilibrium systems from physicochemical data. *TASK Quarterly*, **1998**, 2, 55-72.

Review articles in ISI journals

10. **A. Liwo**, Y. He, H.A. Scheraga. Coarse-grained force field: general folding theory. *Phys. Chem. Chem. Phys.*, **2011**, 13, 16890-16901.

9. A. Lewandowska, S. Ołdziej, **A. Liwo**, H.A. Scheraga. β-hairpin-forming peptides; models of early stages of protein folding. *Biophys. Chem.*, **2010**, 151, 1-9.

8. **A. Liwo**, C. Czaplewski, S. Ołdziej, H.A. Scheraga. Computational techniques for efficient conformational sampling of proteins. *Curr. Opinion. Struct. Biol.*, **2008**, 18, 134-139.

7. H.A. Scheraga, M. Khalili, **A. Liwo**. Protein-folding dynamics: Overview of molecular simulation techniques. *Annu. Rev. Phys. Chem.*, **2007**. 58, 57-83.

6. H.A. Scheraga, **A. Liwo**, S. Ołdziej, C. Czaplewski, J. Pillardy, D. R. Ripoll, J. A. Vila, R. Kazmierkiewicz, J. A. Saunders, Y. A. Arnautova, A. Jagielska, M. Chinchio, M. Nanias. The protein folding problem: global optimization of force fields. *Frontiers in Bioscience*, **2004**, 9, 3296-3323.

5. J. Malicka, C. Czaplewski, M. Groth, W. Wiczk, S. Ołdziej, L. Łankiewicz, J. Ciarkowski, **A. Liwo**. Use of NMR and fluorescence spectroscopy as well as theoretical conformational analysis in conformation-activity studies of cyclic enkephalin analogues. *Current Topics in Medicinal Chemistry*, **2004**, 4, 123-133.

4. H.A. Scheraga, J. Pillardy, **A. Liwo**, J. Lee, C. Czaplewski, D.R. Ripoll, W.J. Wedemeyer, Y.A. Arnautova. Evolution of physics-based methodology for exploring the conformational energy landscape of proteins. *J. Comput. Chem.*, **2002**, 23, 28-34.

3. H.A. Scheraga, J. Lee, J. Pillardy, Y.-J. Ye, **A. Liwo**, D.R. Ripoll. Surmounting the multiple-minima problem in protein folding. *J. Global Optimization*, **1999**, 15, 235-260.

2. **A. Liwo**, S. Ołdziej, R. Kaźmierkiewicz, M. Groth, C. Czaplewski. Design of a knowledge-based force field for off-lattice simulations of protein structure. *Acta Biochim. Pol.*, **1997**, 44, 527-548.

1. M. Tarnowska, **A. Liwo**, F. Kasprzykowski, L. Łankiewicz, J. Ciarkowski. Some aspects of the structure-activity relationships in oxytocin and vasopressin. *Curr. Topics in Med. Chem.*, **1993**, 1, 145-154.

Review articles in non-ISI journals

2. P. Arłukowicz, E. Biernat, J. Ciarkowski, C. Czaplewski, M. Groth, R. Kaźmierkiewicz, **A. Liwo**, K. Maksimiak, M. Nowacka, S. Ołdziej, S. Rodziewicz, E. Woźniak. Molecular simulations with high-performance computers. *TASK. Quarterly*, **1997**, 1, 21-37.

1. **A. Liwo**, M. Tarnowska, J. Ciarkowski, Z. Grzonka. Application of Free-Wilson method in structure-activity correlation of bioactive compounds based on the example of oxytocin and vasopressin analogs. *Wiad. Chem.*, **1994**, **48**, 805-815.

Book chapters

16. A. V. Rojas, G. G. Maisuradze, H. A. Scheraga, **A. Liwo**. Probing Protein Aggregation Using the Coarse-Grained UNRES Force Field. *Computer Simulations of Aggregation of Protein and Peptides: Methods and Protocols*, ed. M.S. Li, A. Kloczkowski, M. Cieplak, M. Kouza, Springer, **2022**, pp 79-104.

15. A. K. Sieradzan, C. Czaplewski, P. Krupa, M. A. Mozolewska, A. Karczyńska, A. Lipska, E. A. Lubecka, E. Gołaś, T. Wirecki, M. Makowski, S. Ołdziej, **A. Liwo**. Modeling the structure, dynamics, and transformations of proteins with the UNRES force field. *Methods in Molecular Biology*, vol. 2376, ed. V. Muñoz, Springera New York, 2022, Chapter 23, pp. 399-416.

14. **A. Liwo**, A. K. Sieradzan, A. S. Karczyńska, E. A. Lubecka, S. A. Samsonov, C. Czaplewski, P. Krupa, M. Mozolewska. Physics-based coarse-grained modeling in bio- and nanochemistry. *Practical Aspects of Computational Chemistry V*, ed. J. Leszczynski, M. Shukla, Springer, **2021**, Chapter 2, pp. 31-69.

13. **A. Liwo**, C. Czaplewski, A.K. Sieradzan, E.A. Lubecka, A.G. Lipska, Ł. Golon, A. Karczyńska, P. Krupa, M.A. Mozolewska, M. Makowski, R. Ganzynkowicz, A. Giełdoń, M. Maciejczyk. Scale-consistent approach to the derivation of coarse-grained force fields for simulating structure, dynamics, and thermodynamics of biopolymers. *Progress in Molecular Biology and Translational Science*, Volume 170, B. Strodel and B. Barz (ed.), Elsevier, 2020.

12. **A. Liwo**, A. K. Sieradzan, C. Czaplewski. Formation of Secondary and Supersecondary Structure of Proteins as a Result of Coupling Between Local and Backbone-Electrostatic Interactions: A View Through Cluster-Cumulant Scope. In: *Protein Supersecondary Structures.* Alexander E. Kister (Ed.), pp. 133-146, Humana Press, Springer, N.Y., 233 Spring Street, New York, NY 10013, U.S.A., 2-10. pp. 133-146.

11. E.I. Gołaś, M.A. Mozolewska, P. Krupa, C. Czaplewski, H.A. Scheraga, **A. Liwo**, Use of Coarse-Grained and All-Atom Molecular Dynamics to Study Hsp70 and Hsp40 Chaperone Action, In: *Role of Molecular Chaperones in Structural Folding, Biological Functions, and Drug Interactions of Client Proteins Book Series: Frontiers in Structural Biology*, Mario D. Galigniana (Ed.), Vol. 1, pp. 23-46, Bentham Science, 2018, eISBN: 978-1-68108-615-6, 2018 ISBN: 978-1-68108-616-3, ISSN: 2589-4366 (Print), ISSN: 2589-4374 (Online).

10. **A. Liwo**, C. Czaplewski, S. Ołdziej, B. Zaborowski, D. Jagieła, J. Lee. Chemoinformatics Methods for Studying Biomolecules. J. Leszczynski et al. (eds.), *Handbook of Computational Chemistry*, Part IV: Biomolecules, Jerzy Leszczynski, Anna Kaczmarek-Kedziera, Tomasz Puzyn, Manthos G. Papadopoulos, Heribert Reis, Manoj K. Shukla, eds., pp 2183-2199, DOI 10.1007/978-94-007-6169-8_56-1, Springer, 2017.

9. M. Baranowski, C. Czaplewski, E. Gołaś, Y. He, D. Jagieła, P. Krupa, **A. Liwo**, G.G. Maisuradze, M. Makowski, M.A. Mozolewska, A. Niadzvedtski, A.J. Niemi, S. Rackovsky, R. Ślusarz, A.K. Sieradzan, S. Ołdziej, T. Wirecki, Y. Yin, B. Zaborowski, H.A. Scheraga, "Microscopic physics-based models of proteins and nucleic acids: UNRES and NARES", in *Coarse-Grained Models of Biomolecules*, ed. by Garegin A. Papoian, CRC Press, ISBN 9781466576063, CAT# K16726, 2017.

8. **A. Liwo**, A. Niemi, X. Peng, A.K. Sieradzan, A novel coarse-grained description of protein structure and folding by UNRES force field and discrete nonlinear Schrödinger equation, in *Frontiers in Computational Chemistry*, ed. by Zaheer-ul-Haq and J. D. Madura, Vol. 1, pp. 257-289, Bentham Science Publishers, 2015.

7. S. Ołdziej, C. Czaplewski, **A. Liwo**, J.A. Vila, H.A. Scheraga, "Computation of structure, dynamics, and thermodynamics of proteins", in E. Engelman (ed) *Comprehensive Biophysics*, Vol. 1 *Biophysical Techniques for Structural Characterization of Macromolecules*, ed. J. Dyson, Oxford: Academic Press, 2014, pp. 494-513.

6. C. Czaplewski, **A. Liwo**, M. Makowski, S. Ołdziej, H.A. Scheraga, "Coarse-grained models of proteins: theory and applications", in A. Kolinski (ed) "Multiscale Approaches to Protein Modeling", Springer, 2010.

5. C. Czaplewski, **A. Liwo**, H.A. Scheraga. "Hydrophobic interactions and protein folding". In *Thermodynamics of Amino Acid and Proein Solutions*, ed. J. Tsurko, W. Kunz, Transworld Research Network, Kerala, India, 2010, pp. 1-18.

4. D.R. Ripoll, **A. Liwo**, H.A. Scheraga. "Global optimization in protein folding". In *Encyclopedia of Global Optimization*,LE-TeX Jelonek, Schmidt & Vöckler GbR, **2008**, pp. 1391-1411.

3. **A. Liwo**, C. Czaplewski, S. Ołdziej, A.V. Rojas, R. Kaźmierkiewicz, M. Makowski, R.K. Murarka, H.A. Scheraga. "Simulation of protein structure and dynamics with the coarse-grained UNRES force field". In: *Coarse-Graining of Condensed Phase and Biomolecular Systems.*, ed. G. Voth, Taylor & Francis, 2008, Chapter 8, pp. 107-122.

2. H.A. Scheraga, **A. Liwo**, S. Ołdziej, C. Czaplewski, J. Pillardy, J. Lee, D.R. Ripoll, J.A. Vila, R. Kaźmierkiewicz, J.A. Saunders, Y.A. Arnautova, K.D. Gibson, A. Jagielska, M. Khalili, M. Chinchio, M. Nanias, Y.K. Kang, H. Schefroth, A. Ghosh, R. Elber, M. Makowski. "The protein folding problem". in New algorithms for macromolecular simulation – Lecture Notes in Computational Science and Engineering, ed. B. Leimkuhler, C. Chipot, R. Elber, A. Laaksonen, A. Mark, T. Schlick, C. Schütte, R. Skeel, Springer, Berlin, 2006.

1. S. Talluri, J.S.R. Murthy, **A. Liwo**, "Structural bioinformatics", in Fundamentals of Bioinformatics, ed. I.A. Khan i A. Khanum, Ukaaz Publications, Hyderabad, India, 2003, pp. 45-90.

Books edited

1. *Computational methods to study the structure and dynamics of biomolecules and biomolecular processes*, ed. by A. Liwo, Springer, Heidelberg, 2014, ISBN 978-3-642-28553-0, 2nd edition 2018.

Papers in conference proceedings

36. S. Ołdziej, C. Czaplewski, **A. Liwo**, H.A. Scheraga, Towards Temperature Dependent Coarse-grained Potential of Side-chain Interactions for Protein Folding Simulations, BIBE, pp.263-266, 2010 IEEE International Conference on Bioinformatics and Bioengineering, 2010

35. I. Liepina, S. Ventura, C. Czaplewski, **A. Liwo**. Dynamics study on single and multiple β-sheets. Peptides for Youth, Book Series: Advances in Experimental Medicine and Biology, Vol. 611, pp. 293-294.

34. **A. Liwo**, C. Czaplewski, S. Ołdziej, U. Kozłowska, M. Makowski, S. Kalinowski, R. Kaźmierkiewicz, H. Shen, G. Maisuradze, H.A. Scheraga, Optimization of a physics-based united-residue force field (UNRES) for protein folding simulations, NIC Series, NIC Symposium 2008, eds. G. Müster, D. Wolf and M. Kremer, **2008**, 39, 63-70.

33. S. Rodziewicz-Motowidło, A. Skwierawska, S. Ołdziej, W. Wiczk, **A. Liwo**, H.A. Scheraga, Conformational studies of a short peptide corresponding to the C-terminal β-hairpin structure of the B1 domain of protein G. *Peptides 2006*, K. Rolka, P. Rekowski and J. Silberring (eds), Kenes, Geneva **2007**, 794-795.

32. I. Liepiņa, S. Ventura, C. Czaplewski, **A. Liwo**. Molecular dynamics study of two Abl-SH3 domain peptides towards amyloid formation. *Peptides 2006*, K. Rolka, P. Rekowski and J. Silberring (eds), Kenes, Geneva **2007**, 782-783.

31. J. Makowska, K. Bagińska, M. Makowski, **A. Liwo**, L. Chmurzyński. Evaluation of two theoretical methods to estimate potentiometric-titration curves of peptides: comparison with experiment. *Peptides 2006*, K. Rolka, P. Rekowski and J. Silberring (eds), Kenes, Geneva **2007**, 62-63.

30. M. Makowski, E. Sobolewski, **A. Liwo**, J. Makowska, L. Chmurzyński, H.A. Scheraga. Determination of potentials of mean force dependent on orientation in hydrophobic systems modeling side-chains of biomolecules. *Peptides 2006*, K. Rolka, P. Rekowski and J. Silberring (eds), Kenes, Geneva **2007**, 60-61.

29. I. Liepiņa, S. Ventura, C. Czaplewski, **A. Liwo**. Multiple β-sheet molecular dynamics of two Abl-SH3 domain peptides. NIC series, NIC Workshop 2007, From Computational Physics to System Biology, Ulrich H.E. Hansmann, Jan Meinke, Sandipan Mohanty, Olav Zimmermann (Editors), Volume 36, pp. 215-218.

28. **A. Liwo**, C. Czaplewski, S. Ołdziej, M. Chinchio, A.V. Rojas, M. Khalili, M. Makowski, S. Kalinowski, U. Kozłowska, R.K. Murarka, H.A. Scheraga. Mesoscopic dynamics with the UNRES force field – a tool for studying the kinetics and thermodynamics of protein folding. NIC series, NIC Workshop 2007, From Computational Physics to System Biology, Ulrich H.E. Hansmann, Jan Meinke, Sandipan Mohanty, Olav Zimmermann (Editors), Volume 36, pp. 31-36.

27. M. Makowski, **A. Liwo**, K. Maksimiak, J. Makowska, L. Chmurzyński, H.A. Scheraga. Simple physics-based analytical formulas for the potentials of mean force for the interaction for amino-acid side chains in water. Tests with simple spherical systems. NIC series, NIC Workshop 2006, From Computational Physics to System Biology, Ulrich H.E. Hansmann, Jan Meinke, Sandipan Mohanty, Olav Zimmermann (Editors), Volume 24, pp. 111-114.

26. F. Rakowski, P. Grochowski, B. Lesyng, **A. Liwo**, H.A. Scheraga. Symplectic algorithms of molecular dynamics. An application to the united-residue model. NIC series, NIC Workshop 2006, From Computational Physics to System Biology, Ulrich H.E. Hansmann, Jan Meinke, Sandipan Mohanty, Olav Zimmermann (Editors), Volume 24, pp. 181-184.

25. U. Kozłowska, K. Wachucik, **A. Liwo**, H.A. Scheraga. Determination of short-range potentials for physics-based protein structure prediction. NIC series, NIC Workshop 2006, From Computational Physics to System Biology, Ulrich H.E. Hansmann, Jan Meinke, Sandipan Mohanty, Olav Zimmermann (Editors), Volume 24, pp. 169-172.

24. **A. Liwo**, M. Khalili, C. Czaplewski, S. Kalinowski, S. Ołdziej, H.A. Scheraga. Optimization of the united-residue UNRES force field for Langevin dynamics simulations. NIC series, NIC Workshop 2006, From Computational Physics to System Biology, Ulrich H.E. Hansmann, Jan Meinke, Sandipan Mohanty, Olav Zimmermann (Editors), Volume 24, pp. 107-109.

23. I. Liepiņa, S. Ventura, C. Czaplewski, **A. Liwo**. Molecular dynamics study of amyloid formation of two Abl-SH3 domain peptides. NIC series, NIC Workshop 2006, From Computational Physics to System Biology, Ulrich H.E. Hansmann, Jan Meinke, Sandipan Mohanty, Olav Zimmermann (Editors), Volume 24, pp. 103-106.

22. C. Czaplewski, S. Kalinowski, S. Ołdziej, **A. Liwo**, H.A. Scheraga. Multiplexed replica exchange molecular dynamics with the UNRES force field as an effective method for exploring conformational energy landscape of proteins. NIC series, NIC Workshop 2006, From Computational Physics to System Biology, Ulrich H.E. Hansmann, Jan Meinke, Sandipan Mohanty, Olav Zimmermann (Editors), Volume 24, pp. 63-66.

21. H.A. Scheraga, **A. Liwo**, St. Ołdziej, C. Czaplewski, M. Khalili, J.A. Vila, D.R. Ripoll. The two aspects of the protein folding problem. NIC series, NIC Workshop 2006, From Computational Physics to System Biology, Ulrich H.E. Hansmann, Jan Meinke, Sandipan Mohanty, Olav Zimmermann (Editors), Volume 24, pp. 37-44.

20. J. Łągiewka, S. Rodziewicz-Motowidło, R. Sosnowska, K. Stachowiak, S. Ołdziej, **A. Liwo**, Z. Grzonka. Investigation of the hCC dimerization mechanism – CD and NMR structural stability studies of the β2-L1-β3 fragment. *Peptides 2004*, M. Flegel, M. Fridkin, C. Gilon, J. Slaninova (eds.), Keynes, Geneva, **2005**, 1029-1030.

19. I. Liepiņa, P. Janmey, C. Czaplewski, **A. Liwo**. Towards gelsolin amyloid formation. *Peptides 2004*, M. Flegel, M. Fridkin, C. Gilon, J. Slaninova (eds.), Keynes, Geneva, **2005**, 740-741.

18. J. Ciarkowski, P. Drabik, Z. Grzonka, V. Hruby, **A. Liwo**, S. Ołdziej, E. Politowska, M.D. Shenderovich, M. Witt. From modeling neurohypophyseal hormones to signaling mechanisms in GCPRs. *Peptides 2004*, M. Flegel, M. Fridkin, C. Gilon, J. Slaninova (eds.), Keynes, Geneva, **2005**, 125-127.

17. I. Liepina, P. Janmey, C. Czaplewski, **A. Liwo**. Molecular dynamics of the caspase-3 cleaved N-half of gelsolin. *Biopolymers*, **2003**, 71, 331.

16. I. Liepiņa, C. Czaplewski, P. Janmey, **A. Liwo**. Molecular dynamics of the gelsolin-derived peptide binding to a PIP_2-containing lipid bilayer. *Peptides 2000*, J. Martinez and J.-A. Fehrentz (eds.), EDK, Paris, **2001**, 987-988.

15. S. Rodziewicz-Motowidło, K. Brzozowski, A. Łęgowska, **A. Liwo**, K. Rolka, J. Silbering, M. Smoluch. Conformational studies of neuropeptide γ using CD, 2D NMR spectroscopy and theoretical analysis. *Peptides 2000*, J. Martinez and J.-A. Fehrentz (eds.), EDK, Paris, **2001**, 459-460.

14. R. Ganzynkowicz, A. Rzeska, **A. Liwo**, W. Wiczk. Influence of a rotamer population on fluorescence decay of the tyrosine derivatives studied by fluorescence, ^{1}HNMR spectroscopy, and theoretical calculation. *Peptides 2000*, J. Martinez and J.-A. Fehrentz (eds.), EDK, Paris, **2001**, 411-412.

13. **A. Liwo**, J. Pillardy, C. Czaplewski, J. Lee, D.R. Ripoll, M. Groth, S. Rodziewicz-Motowidlo, R. Kazmierkiewicz, R.J. Wawak, S. Ołdziej, H.A. Scheraga, UNRES – a united-residue force field for energy-based prediction of protein structure - origin and significance of multibody terms, RECOMB 2000, Proceedings of the Fourth Annual International Conference on Computational Molecular Biology, R. Shamir, S. Miyano, S. Istrail, P. Pevzner, M. Waterman (Eds.), April 8-11, Tokyo, Japan, ACM, New York, pp. 193-200.

12. S. Rodziewicz, I. Wirkus-Romanowska, M. Ciurak, H. Miecznikowska, C. Czaplewski, **A. Liwo**, K. Rolka, G. Kupryszewski. Cyclic analogues of proline-rich protein fragment, synthesis and conformational studies. *Peptides 1998*, S. Bajusz and F. Hudecz (eds.), Akademiai Kiadó, Budapest, **1999**, 448-449.

11. M. Groth, J. Malicka, C. Czaplewski, W. Wiczk, **A. Liwo**. Conformational studies of cyclic enkephalin analogues with L- or D-proline in position 3 by NMR spectroscopy and global

conformational analysis. *Peptides 1998*, S. Bajusz and F. Hudecz (eds.), Akademiai Kiadó, Budapest, **1999**, 370-371.

10. J. Malicka, C. Czaplewski, M. Groth, A. Kubicki, P. Arłukowicz, W. Wiczk, **A. Liwo**. Studies of inter-pharmacophore distance in cyclic enkephalin analogues by fluorescence spectroscopy and molecular dynamics. *Peptides 1998*, S. Bajusz and F. Hudecz (eds.), Akademiai Kiadó, Budapest, **1999**, 368-369.

9. S. Rodziewicz, A. Lesner, K. Rolka, A. Łęgowska, C. Czaplewski, **A. Liwo**, R. Patacchini, L. Quartara. Conformational studies of scyliorhinin II analogues - tachykinin peptides using NMR spectroscopy and Monte Carlo global conformational analysis. *Peptides 1998*, S. Bajusz and F. Hudecz (eds.), Akademiai Kiadó, Budapest, **1999**, 334-335.

8. B. Micewicz, **A. Liwo**, L. Łankiewicz, W. Wiczk. Mechanism of tyrosine fluorescence quenching by acrylamide in model peptides. *Peptides 1996*, Ramage & Epton, (eds.), **1998**, 649-650.

7. M.D. Shenderovich, K.E. Kövér, S. Wilke, M. Romanowski, **A. Liwo**, L. Łankiewicz, E. Gwizdała, J. Ciarkowski, V.J. Hruby. Conformational analysis of potent bicyclic antagonists of oxytocin: NMR, CD and molecular dynamics study. *Peptides 1995*, (Proc. 14th APS), Kaumaya, P.T.P. and Hodges, R.S., Eds., Mayflower Scientific Ltd., England **1996**, 499-500.

6. J. Ciarkowski, S. Ołdziej, M. Nowacka, **A. Liwo**, F.M.F. Chen, and L. Benointon. Mixed anhydride reactivity by means of the molecular orbital AM1 and PM3 methods. *Peptides 1994*, ed. H.L.S. Maia, ESCOM, Leiden 1995, pp. 213-214.

5. M. Tarnowska, **A. Liwo**, Z. Grzonka, A. Tempczyk. Modified Free-Wilson analysis of the neurohypophyseal hormone analogs II: Analogs of oxytocin-like activity. In *QSAR in Design of Bioactive Compounds*, Vol. 2, ed. M. Kuchar, J.R. Prous Science Publishers: Barcelona 1991, pp. 399-436.

4. M. Tarnowska, **A. Liwo**, Z. Grzonka, A. Tempczyk. Modified Free-Wilson analysis of the neurohypophyseal hormone analogs I: Analogs of vasopressin-like activity. In *QSAR in Design of Bioactive Compounds*, Vol. 2, ed. M. Kuchar, J.R. Prous Science Publishers: Barcelona 1991, pp. 361-397.

3. S. Ołdziej, F. Kasprzykowski, L. Łankiewicz, P. Kania, **A. Liwo** and Z. Grzonka. Proposed mechanism of interaction of type II cystatins with papain. In *Peptides 1991*, eds. J.A. Smith, J.E.Rivier, ESCOM, Leiden 1991, pp. 793-794.

2. Z. Grzonka, E. Gwizdała, F. Kasprzykowski, **A. Liwo**, L. Łankiewicz, L. Łubkowska, S.G. Galaktionov, V.M. Tseitsin. Studies on interaction of neurohypophyseal hormones with lipids. In *Peptides 1990*, eds. E. Ginolt, D. Andrew, ESCOM, Leiden 1991, pp. 488-489

1. F. Kasprzykowski, P. Kania, S. Ołdziej, **A. Liwo**, M. Tarnowska, Z. Grzonka, M. Abrahamson, I. Olafsson, A. Grubb and J. Trojnar. Inhibition of cysteine proteinases by a series of peptidyl-diazomethanes structurally related to the binding center of cystatins. In *Peptides 1990*, eds. E. Ginolt, D. Andrew, ESCOM, Leiden 1991, pp. 799-800.

Józef Adam Liwo

Invited presentations

50. Long-time dynamics of selected molecular-motor components using a physics-based coarse-grained approach. 21th KIAS Conference on Protein Structure and Function, Seoul, South Korea, October 11 – 14, 2023.

49. Long-time dynamics of selected molecular-motor components using a physics-based coarse-grained approach. 7th Telluride Workshop on Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules, July 24 – 28, 2023, Telluride, USA.

48. Recent developments and applications of the UNICORN coarse-grained model of biological macromolecules. Workshop on Topology, Physics, and Chemistry of Soft Matter: Eutopia IV, 5 – 9 September 2022, Trento, Italy.

47. Origin of through-sequence correlations between local conformational states of amino-acid residues and their role in shaping protein structures and in allostery. 20th KIAS Conference on Protein Structure and Function, Seoul, South Korea, September 14 – 17, 2022.

46. Origin of through-sequence correlations between local conformational states of amino-acid residues and their role in shaping protein structures and in allostery. 6th Telluride Workshop on Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules, July 25 – 28, 2022, Telluride, USA.

45. Theory and practice of coarse graining, Mathematics of Life, MoL2021, 13 – 16 September 2021, Hisarya, Bulgaria & online.

44. Data-assisted modeling of protein structures with the coarse-grained UNRES model . 14th Community Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction CASP14, Virtual Meeting, November 30 – December 4, 2020.

43. The Unified Coarse Grained model of biological macromolecules: principles and applications. XLVIII Annual Meeting of the Argentinian Biophysical Society, San Luis, Argentina, Nov. 27 – 29, 2019.

42. The scale-consistent UNICORN package for large-scale simulations of biological macromolecules. E-CAM Extended Software Development Workshop: Inverse Molecular Design & Inference: building a Molecular Foundry I, Clifden, Galway, Ireland, November 1 – 9, 2019.

41. A scale-consistent approach to coarse graining biomolecular systems. The 19th KIAS Conference on Protein Structure and Function, Korea Institute for Advanced Study, Seoul, Korea, September 26-September 28, 2019.

40. New scale-consistent UNRES force field for protein simulatios. CECAM Protein Simulations – Current State of Art, Tel Aviv, Israel, October 22-24, 2019.

39. Simulations of protein structure, dynamics, and thermodynamics with the coarse-grained UNRES force field and massively parallel computers. HPC 2019 Bulgaria, September 2-6, 2019, Borovets, Bulgaria.

38. Physics-based scale- and geometry-consistent coarse-grained potentials. Workshop on Multiscale Modelling, Leiden, The Netherlands, June 24-June 28, 2019.

37. Using the UNRES server and the standalone UNRES package in SAXS-data-assisted modeling of protein structure. simSAS 2019, Grenoble France, April 8-11/12, 2019

36. Data-assisted prediction of protein structures with the coarse-grained UNRES force field. CASP13 Meeting, Iberostar Paraiso Maya, Mexico, December 1-4, 2018.

35. Physics-based scale- and geometry-consistent coarse-grained potentials. 26th Conference on Current Trends in Computational Chemistry (2018 CCTCC) Jackson, MS (USA), 9-10 November 2018.

34. Systematic design of physics-based scale-consistent coarse-grained potentials for the simulations of biomolecules and nanostructures, Bio-, chem-, and nanoinformatics approaches to study bionano interface Dublin, Ireland, May 23-25, 2018.

33. Implementation of geometry-consistent local and correlation potentials in the UNRES force field. Biomolecules and Nanostructures 6, Podlesice, Poland, May 10-14, 2017

32. Geometry-consistent expressions for energy terms in coarse-grained force fields for (bio)polymers with UNRES as an example. Workshop on Physics and Biology of Proteins, Natal, Brazil, June 12-30, 2017

31. A general method for the derivation of effective energy expressions in coarse-grained force fields. 3rd Korean-Polish Conference on Protein Folding: Theoretical and Experimental Approaches, Seoul, Republic of Korea, February 4 9, 2017

30. The Unified Coarse-Grained Model for large-scale simulations of biological macromolecules. The 16th KIAS Conference on Protein Structure and Function, Seoul, Republic of Korea, September 22 – September 24, 2016.

29. How do the local and long-range interactions encode the three-dimensional structures of biological macromolecules: a coarse-grained perspective. 6th Visegrad Symposium on Structural Systems Biology, Warsaw, Poland, 19-21 June, 2016.

28. A rigorous approach to derive analytical expressions for the effective energy terms in coarse-grained force fields. 3rd International Conference on Protein and RNA Structure Prediction Punta Cana, Dominican Republic, Dec 14-18, 2015.

27. The UNRES coarse-grained model of polypeptide chains: theory and applications. Invited lecture presented at the Department of Physics, Beijing Institute of Technology, Beijing, P.R. China, September 17, 2015.

26. Maximum-likelihood calibration of force fields. 1st Korean-Polish Conference on Protein Folding: Theoretical and Experimental Approaches, Seoul, Rep. of Korea, May 24-28, 2015.

25. A unified coarse-grained model for biomolecular simulations. 2015 Workshop of Wuhan Center of Physical Biology, Wuhan, P.R. China, September 7, 2015.

24. A rigorous approach to the derivation of analytical potentials in physics-based coarse-grained force fields. 3rd International Workshop on Theoretical and Computational Physics, Complex Systems and Interdisciplinary Physics, Da Lat, Vietnam, July 27-30, 2015.

23. The first Nobel Prize in computational chemistry. An invited lecture presented during the quarterly Colloquium at the Inistitute of Physics, Polish Academy of Sciences, Warsaw, Poland, February 25, 2014.

22. A maximum-likelihood approach to force-field calibration. Protein Folding Conference 2014, Grand Palladium Resort & Spa, Bavaro Hotel Punta Cana, Dominican Republic, July 16-19, 2014.

21. Essential role of mean-field electrostatic interactions in free modeling of protein and nucleic acid structures at coarse-grained level. Protein & RNA Structure Prediction Conference 2013, Occidental Grand Xcaret, Playa del Carmen Mexico, December 1-5, 2013.

20. Mean field dipole-dipole interactions as essential factors in the formation of biomolecular architectures. Biomolecules and Nanostructures 4, Pułtusk, Poland, May 15-19, 2013.

19. A simple coarse-grained model of nucleic acids reveals the essential role of mean-field dipole-dipole interactions between nucleic-acid bases and double-helix formation. Fifth Korea-Japan Seminars on Biomolecular Sciences: Experiments and Simulations. High1 Resort, Republic of Korea, February 24-16, 2013.

18. Coarse grained description of biomolecular systems. 10th Workshop on Bioinformatics and 5th Symposium of the Polish Bioinformatics Society, Gdańsk, Poland, May 25-26, 2012.

17. Coarse-grained models for proteins. Nordita Workshop "Dynamics of Biomolecular Processes: From Atomistic Representations to Coarse-Grained Models", Stockholm, Sweden, February 27 - March 23, 2012; a series of 4 invited lectures.

16. Construction and application of coarse-grained force fields for biomacromolecules, Multipole Approaches to Structural Biology, Warsaw, Poland, November 16-19, 2011.

15. From atomistic simulations to network description of biological systems, Workshop "From Computational Biophysics to Systems Biology" 2011 (CBSB11), Juelich, Germany, July 20-22, 2011.

14. The nature of the conformational ensemble at the transition temperature: insights from simulations and experiment. Third Korea-Japan Seminars on Biomolecular Sciences: Experiments and Simulations, Hotel Lotte, Jeju, Korea, February 26, March 1, 2011.

13. Use of the UNRES force field and massively parallel computers in millisecond scale simulations of protein dynamics. Workshop on Bioinformatics (BIT09), Toruń, Poland May 23-25, 2009.

12. Towards simulations of structure and dynamics of large proteins with the UNRES force field. The 8th KIAS - Yonsei Conference on Protein Structure and Function, Seoul, Korea, October 9-11, 2008.

11. Prediction of structure and simulation of dynamics of protein folding with the mesoscopic UNRES force field, Modelling and Design of Molecular Materials. Piechowice, Poland, June 23-28, 2008.

10. Mesoscopic dynamics with the UNRES force field - a tool for studying the kinetics and thermodynamics of protein folding. NIC Workshop 2007, From Computational Biology to System Biology, Jülich, Germany, May 2-4, 2007.

9. Optimization of a mesoscopic force field for simulation of protein folding pathways. Workshop on Structure and Function of Biomolecules May 13-15, 2006, Będlewo near Poznań, Poland.

8. Ab initio simulations of protein folding pathways by molecular dynamics with the united-residue (UNRES) model of polypeptide chains. 30th FEBS Congress and 9th IUBMB Conference, Budapest, Hungary, 2005; FEBS Journal., **2005**, 272 (Suppl. 1) 359.

7. Design of hierarchical caldera-like potential-energy functions for energy-based prediction of protein structure and simulation of protein folding:application to the UNRES force field. Third KIAS Conference on Protein Structure and Function: Folding Mechanism, Proteomics, and Bioinformatics, Seoul, Korea, 29.09-1.10, 2003, 2003,

6. Energy-based prediction of protein structure with the UNRES force field, First KIAS Conference on Protein Structure and Function: Protein Folding in Post-Genome Era, Korea Institute for Advanced Study, Seoul, Korea, November 28 - November 30, 2001.

5. A knowledge-based united-residue force field for off-lattice calculations of protein structure that recognizes native folds. International Symposium on Theoretical, Experimental Aspects of Protein Folding, San Luis, Argentina, June 17-21, 1996

4. Role of singlet-oxygen binding to anthraquinones in the peroxidating activity of antitumor anthraquinone drugs. 5th International Symposium on Molecular Aspects of Chemotherapy, Gdansk, Poland, August 21-24, 1995

3. Prediction of protein structure using a mean-field united-residue potential determined from protein crystal data. 3-rd Conference Computers in Chemistry '94, Wrocław, Poland, June 23-26, 1994.

2. Application of the Free-Wilson method in structure-activity correlation of bioactive compounds on the example of oxytocin and vasopressin analogs. Theoretical and Experimental Aspects of Molecular Structure, Karpacz, Poland, June 5-10, 1994

1. The role of hydrophobic residue packing in protein folding. 8th Conference of Young Scientists on Organic, Bioorganic Chemistry, Riga, Latvia, 2-9 November 1991.