Curriculum vitae

Personal data:

`Name:`	**Jacek Czub**
`Nationality:`	Polish
`Address:`	Department of Physical Chemistry
	Gdansk University of Technology
	ul. Narutowicza 11/12, 80-233 Gdańsk, Poland
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Academic Positions:

- 2016– : associate professor (tenured), Gdansk University of Technology, Department of Physical Chemistry, Gdańsk, Poland
- 2011–2016 : assistant professor, Gdansk University of Technology, Department of Physical Chemistry, Gdańsk, Poland
- 2008–2011 : postdoctoral fellow, Department of Theoretical and Computational Biophysics (supervisor: prof. Helmut Grubmüller), Max Planck Institute for Biophysical Chemistry in Göttingen, Germany

Education:

- 2003–2008: PhD student, Gdansk University of Technology, Department of Pharmaceutical Technology and Biochemistry, PhD degree in Chemistry
- 1997–2002: undergraduate student, Gdansk University of Technology, Faculty of Chemistry, specialization: Pharmaceutical Biotechnology, MSc degree in Biotechnology

Research Interests:

- in general: application of theoretical and computational methods to study (bio)molecular systems; computer-aided drug design; computation of free energy differences using molecular simulations, design and implementation of computational methods
- more specifically:
  - mechanism of energy transmission and conversion in the F_OF_1-ATP synthase
  - structural and dynamic properties of membrane-bound molecules and membrane proteins
  - conformational dynamics and allosteric control in the Hsp70 chaperone proteins
  - protein-DNA interactions with a special emphasis on telomeric region of chromosomes
  - solvation of biological biomacromolecules; effect of osmolytes on stability of proteins and DNA
  - molecular properties of G-quadruplexes—non-canonical DNA motifs

Professional activities

- Teaching experience:

  - Physical Chemistry (full course)
  - Computer Science (full course)
  - Mathematical Methods in Chemistry (full course)
  - Spectroscopic Methods in Organic Chemistry (laboratories)
  - Numerical Methods for Chemists (practical works)
  - Elements of Computer Science and Bioinformatics (computer laboratories)

- Supervision/co-supervision of PhD students (Beata Adamczak, Mateusz Kogut, Lidia Chomicz, Łukasz Nierzwicki, Miłosz Wieczór, Cyprian Kleist), MSc students (Beata Adamczak, Mateusz Kogut, Adrian Tobiszewski, Łukasz Nierzwicki, Miłosz Wieczór, Kamil Jaworski, Paulina Gdaniec, Judyta Harasimowicz, Cyprian Kleist, Jakub Jurasz) and BSc students (Diana Toczydłowska, Judyta Harasimowicz, Miłosz Wieczór, Paweł Wityk, Łukasz Nierzwicki, Cyprian Kleist, Mateusz Dutkiewicz)

- Served as a reviewer for: Journal of the American Chemical Society, Angewandte Chemie International Edition, Biochemistry, European Biophysics Journal, Journal of Chemical Physics, Journal of Medicinal Chemistry, Biophysical Journal, Cellular Physiology and Biochemistry, Bioconjugate Chemistry, Journal of Physical Chemistry

Honors and Awards:

- merit scholarship from GUT during the entire undergraduate period
- GUT Rector's Award for undergraduate students (1998, 1999, 2000, 2001)
- prize of the Polish Chemical Society for the best MSc thesis defended in 2002 at the Faculty of Chemistry, GUT (2002)
- Regional Scholarship for PhD students (funded by European Social Fund) (2005/2006)
- Scholarship for young investigators awarded by the Foundation for Polish Science ("Start" Programme) (2008)
- research grant within the Foundation for Polish Science "Homing Plus" Programme (2012)
- Scholarship for young investigators awarded by the Ministry of Science and Higher Education (2012–2015)

General skills and competences:

- *programming:* C/C++ (incl. MPI library), Python, TCL, bash, Perl, basic knowledge of Fortran77
- *operating systems:* Linux (user/admin), Linux cluster, Windows
- *software:* extensive knowledge of molecular simulation tools (GROMACS, NAMD, CHARMM, CP2K, Gaussian, VMD, CPMD, Quanta, InsightII, MOPAC, GAMESS, AMBER, AutoDock Vina, APBS etc.) and other scientific packages (Mathematica, Matlab, LaTeX, SigmaPlot, graphical software, etc.)
- *languages:* Polish–native, English–fluent (written/oral), Russian–basic

Research grants:

- As a principal investigator

  - research project funded by the Ministry of Science and Higher Education within the within Iuventus Plus programme (IP2012 03472), "Mechanism of energy conversion in catalytic sector of ATP synthase", 2013–2016, principal investigator
  - research project funded by the Foundation for Polish Science within the Homing Plus programme (HOMING PLUS/2011-4/3), "Telomeres as targets for anticancer drug development – a computational approach", 2012–2014„ principal investigator

- As an investigator/advisor
  - The Polish Committee of Scientific Research targeted project (6 T11 2003 C/06098), "CLUSTERIX – the National Linux Cluster", task 14: Adapting applications to a grid environment, 2003–2005, investigator
  - research project funded by the Polish Committee of Scientific Research (KBN 3 P05F 012 25), "Computer-aided design of new antifungal agents polyene macrolides and inhibitors of glucosamine-6-phosphoran synthase", 2003–2007, PI: prof. Maciej Bagiński, main investigator
  - research project funded by the Polish Committee of Scientific Research (N519 035 32/4168), "Molecular modelling studies on the mechanism of action of amphotericin B and its more selective derivatives", 2007–2008, PI: prof. Maciej Bagiński, main investigator
  - research project funded by the Ministry of Science and Higher Education (N301 121 32/4127), "Complexes of TRF1 and TRF2 proteins with telomeric DNA ad their evaluation as potential anticancer drug targets", PI: prof. Maciej Bagiński, 2007–2011; investigator
  - research project funded by the polish National Science Center within the OPUS programme (UMO-2013/11/B/NZ1/02258) "Stability of proteins in aqueous osmolyte solutions – a combined experimental-computational approach", PI: prof. Janusz Stangret, 2014–2017; main investigator
  - research project funded by the Ministry of Science and Higher Education within the "Diamantowy grant" programme (0059/DIA/2014/43), "Molecular mechanism of the effect of oxidative stress on the structral stability and dynamics of the complexes of telomeric DNA with proteins", PI: Miłosz Wieczór, scientific advisor
  - research project funded by the polish National Science Center within the MAESTRO programme (UMO-2014/14/A/ST4/00405), "From a molecular in silico model to cellular response in vitro Modified nucleosides as photo and/or radiosensitizers of DNA damage", PI: prof. Janusz Rak (UG), 2015–2019; investigator

Hobbies:
Experimental and contemporary music, philosophy and history of science, literature

References:

Dr hab. inż. Maciej Bagiński, Wydział Chemiczny, Politechnika Gdańska
ul. Narutowicza 11/12, 80-233 Gdańsk, Polska.
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Prof. dr hab. inż. Janusz Stangret, Wydział Chemiczny, Politechnika Gdańska
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Prof. Helmut Grubmueller, Max Planck Institute for Biophysical Chemistry, Department of Theoretical and Computational Biophysics

Am Fassberg 11, D-37077 Goettingen, Germany.
Email: hgrubmu@gwdg.de, Tel: +49 551 201 2301

Prof. Janusz Rak, Wydział Chemii, Uniwersytet Gdański
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Email: janusz.rak@ug.edu.pl Tel: +48 58 523 51 18

List of Publications:

1. M. Wieczor, **J. Czub***
   How proteins bind to DNA: target discrimination and dynamic sequence search by the telomeric protein TRF1
   Nucleic Acids Res. 13:7643–7654 (2017)

2. J. Pilipczuk, B. Zalewska-Piatek, P. Bruzdziak, **J. Czub**, M. Wieczor, M. Olszewski, M. Wanarska, B. Nowicki, D. Augustin-Nowacka, R. Piatek
   Role of the disulfide bond in stabilization and folding of the fimbrial protein DraE
   J. Biol. Chem. (2017) *in press*

3. W. Grudzinski , L. Nierzwicki, R. Welc, E. Reszczynska, R. Luchowski, **J. Czub***, W.I. Gruszecki
   Localization and Orientation of Xanthophylls in a Lipid Bilayer.
   Sci. Rep. 7: 9619 (2017)

4. **J. Czub**, M. Wieczor, B. Prokopowicz, H. Grubmüller.
   Mechanochemical Energy Transduction during the Main Rotary Step in the Synthesis Cycle of F1-ATPase.
   J. Am. Chem. Soc. 139:4025–4034 (2017)

5. B. Adamczak, M. Wieczor, M. Kogut, J. Stangret, **J. Czub***.
   Why is betaine excluded from and urea accumulated at the protein surface? An insight into the cosolvent effect on protein stability from the mechanical unfolding of lysozyme.
   Biochem. J. 473:3705–3724 (2016)

6. K. Szwarc, M. Płosiński, K. Czerniejewska, T. Laskowski, A. Leniak, **J. Czub**, P. Kubica, P. Sowiński, J. Pawlak, E. Borowski.
   Intramolecular transformation of an antifungal antibiotic nystatin A1 into its isomer, iso-nystatin A1. Structural and mechanistic studies.
   Magn. Reson. Chem. 54:953–961 (2016)

7. A. Nowak-Zaleska, M. Wieczor, **J. Czub**, L. Nierzwicki, R. Kotlowski, A. Mikucka, E. Gospodarek.
   Correlation between the number of Pro-Ala repeats in the EmrA-homologue of Acinetobacter baumannii and resistance to Netilmicin, Imipenem, Tobramycin and Ceftazidime.
   J. Glob. Antimicrob. Resist. 7:145–149 (2016)

8. M. Kogut, C. Kleist, **J. Czub***.
   Molecular dynamics simulations reveal the balance of forces governing the formation of a guanine tetrad – a common structural unit of G-quadruplex DNA.
   Nucleic Acids Res. 44:3020–3030 (2016)

9. A. Neumann, M. Wieczor, J. Zielinska, M. Baginski, **J. Czub***.
   Membrane sterols modulate the binding mode of amphotericin B without affecting its affinity for

a lipid bilayer.
Langmuir 32:3452–3461 (2016)

10. T. Laskowski, **J. Czub**, P. Sowinski, J. Mazerski.
NMR studies on the stereochemistry of the imidazoacridinone C-1311 complexes with short fragments of double-stranded DNA, part I: the d(CGATCG)2:C-1311 complex.
J. Biomol. Struct. Dyn. 34:653–663 (2016)

11. W. Delewski, B. Paterkiewicz, M. Manicki, B. Schilke, B. Tomiczek, S. Ciesielski, L. Nierzwicki, **J. Czub**, R. Dutkiewicz, E. A. Craig, J. Marszalek.
Mutational robustness emerged as an intrinsic property of protein interaction network; a case study of J-protein co-chaperone involved in iron-sulfur cluster biogenesis.
Mol. Biol. Evol. 33:643–656 (2016)

12. J. Zielinska, M. Wieczor, T. Baczek, M.Gruszecki, **J. Czub***.
Thermodynamics and kinetics of amphotericin B self-association in aqueous solution characterized in molecular detail.
Sci. Rep. (2015) 6:19109 (2016)

13. P. Bruzdziak, B. Adamczak, E. Kaczkowska, **J. Czub**, J. Stangret.
Are stabilizing osmolytes preferentially excluded from the protein surface? FTIR and MD studies.
Phys. Chem. Chem. Phys. 17:23155–23164 (2015)

14. L. Marcinkowski, A. Kloskowski, **J. Czub**, J. Namiesnik, D. Warminska.
Solvation of ionic liquids based on N-methyl-N-alkyl morpholinium cations in dimethylsulfoxide – volumetric and compressibility studies.
J. Chem. Thermodyn. 88:36–43 (2015)

15. A. Panuszko, B. Adamczak, **J. Czub**, E. Gojlo, J. Stangret.
Hydration of amino acids. FTIR spectra and mlecular dynamics studies.
Amino Acids 47:2265–2278 (2015)

16. L. Nierzwicki, **J. Czub***.
Specific binding of cholesterol to the amyloid precursor protein: structure of the complex and driving forces characterized in molecular detail.
J. Phys. Chem. Lett. 6:784–790 (2015)

17. L. Nierzwicki, M. Wieczor, V. Censi, M. Baginski, L. Calucci, S. Samaritani, **J. Czub***, C. Forte.
Interaction of cisplatin and two potential antitumoral platinum(II) complexes with a model lipid membrane: a combined NMR and MD study.
Phys. Chem. Chem. Phys. 17:1458–1468 (2015)

18. J. Starzyk, M. Gruszecki, K. Tutaj, R. Luchowski, R. Szlazak, P. Wasko, W. Grudzinski, **J. Czub**, W.I. Gruszecki.
Self-association of amphotericin B: Formation of molecular structures responsible for the toxic side effects of the antibiotic.
J. Phys. Chem. B 118:13821–13832 (2014)

19. **J. Czub**, H. Grubmüller.
Rotation Triggers Nucleotide-Independent Conformational Transition of the Empty β Subunit of F_1-ATPase.
J. Am. Chem. Soc. 136:6960–6968 (2014)

20. M. Wieczór, P. Wityk, A. Tobiszewski, B. Tomiczek, **J. Czub***.
Molecular recognition in complexes of TRF proteins with telomeric DNA.
PLoS ONE 9:e89460 (2014)

21. M. Wieczór, P. Wityk, **J. Czub***, L. Chomicz, J. Rak.
First-principles study of electron attachment to the fully hydrated bromonucleobases.
Chem. Phys. Letters 595–596:133–137 (2014)

22. A. Neumann, M. Baginski, S. Winczewski, **J. Czub***.
The effect of sterols on Amphotericin B self-aggregation in a lipid bilayer as revealed by free energy simulations.
Biophys. J. 104:1485–1494 (2013)

23. **J. Czub**, H. Grubmüller.
Torsional elasticity and energetics of F_1-ATPase.
Proc. Natl. Acad. Sci. USA 108:7408–7414 (2011)

24. C. Kutzner, **J. Czub**, H. Grubmüller.
Keep it flexible: driving macromolecular rotary motion in atomistic simulations with GROMACS.
J. Chem. Theory Comput. 7:1381–1393 (2011)

25. A. Neumann, M. Baginski, **J. Czub***.
How do sterols determine the antifungal activity of amphotericin B? Free energy of binding between the drug and its membrane targets.
J. Am. Chem. Soc. 132:18266–18272 (2010)

26. A. Neumann, **J. Czub**, M. Baginski.
On the possibility of the amphotericin B-sterol complex formation in cholesterol- and ergosterol-containing lipid bilayers – a molecular dynamics study.
J. Phys. Chem. B 113:15875–15885 (2009)

27. M. Baginski, **J. Czub**.
Amphotericin B and its new derivatives – chemotherapeutic action.
Curr. Drug Metabolism 10:459–469 (2009)

28. **J. Czub**, A. Neumann, E. Borowski, M. Baginski.
Influence of a lipid bilayer on the conformational behavior of amphotericin B derivatives – a molecular dynamics study.
Biophys. Chem. 141:105–116 (2009)

29. M. Slisz, B. Cybulska, J. Grzybowska, **J. Czub**, R. Prasad, E. Borowski.
Amphotericin B and its derivatives of varied selective toxicity: action on fungal strains containing multidrug transporters.
J. Antib. 60:436–446 (2007).

30. **J. Czub**, E. Borowski, M. Baginski.
Interactions of amphotericin B derivatives with lipid membranes - a molecular dynamics study.
BBA-Biomembranes, 1768:2616–2626 (2007).

31. M. Baginski, **J. Czub**, K. Sternal.
Interaction of Amphotericin B and its selective derivatives with membranes: molecular modeling studies.
Chem. Rec. 6:320–332 (2006).

32. **J. Czub**, M. Baginski.
Modulation of amphotericin B membrane interaction by cholesterol and ergosterol - a molecular dynamics study.
J. Phys. Chem. B 110:16743–16753 (2006).

33. **J. Czub**, M. Baginski.
Comparative molecular dynamics study of lipid membranes containing cholesterol and ergosterol.
Biophys. J. 90:2368–2382 (2006).

34. P. Seroka, M. Plosinski, **J. Czub**, P. Sowinski, J. Pawlak. Monosaccharides as internal probes for the determination of the absolute configuration of 2-butanol.
Magn. Reson. Chem. 44:132–138 (2006).

35. M. Baginski, K. Sternal, **J. Czub**, E. Borowski.
Molecular modelling of membrane activity of amphotericin B, a polyene macrolide antifungal antibiotic.
Acta Biochim. Pol. 52:655–658 (2005).

36. K. Sternal, **J. Czub**, M. Baginski
Molecular aspects of the interaction between amphotericin B and a phospholipid bilayer: molecular dynamics studies.
J. Mol. Model. 10: 223-232 (2004).

* – corresponding author

Conference contributions:

1. M. Wieczór, J. Czub. Target discrimination and dynamic sequence search by the telomeric protein TRF1, July 2017, 11th European Biophysics Congress EBSA, Edinburgh, UK

2. B. Tomiczek, W. Delewski, M. Stolarska, B. Schilke, R. Dutkiewicz, S. J. Ciesielski, L. Nierzwicki, I. Grochowina, **J. Czub**, E. A. Craig, J. Marszalek. Probing molecular mechanisms of J-protein-Hsp70 interaction with chaperones dedicated for iron-sulfur cluster biogenesis. May 2017, EMBO Conference: Protein quality control: Success and failure in health and disease, Sant Feliu de Guixols, Spain

3. J. Rak, L. Chomicz-Mańka, K. Westphal, J. Wiczk, P. Wityk, M. Zdrowowicz, M. Wieczor, **J. Czub**. Hydrated electrons and Trojan horse radiotherapy. Computational and experimental studies. Modeling and Design of Molecular Materials, June 2016; Trzebnica, Poland

4. M. Wieczor, **J. Czub**. Sequence-Specific Binding and Diffusion of TRF1 on Telomeric DNA Studied by Molecular Dynamics. Biophysical Society 60th Annual Meeting, February 2016; Los Angeles, CA, USA; *Biophys. J.* 110(3):645a.

5. **J. Czub**, M. Wieczor, M. Dutkiewicz, H. Grubmüller. Mechanism of Energy Conversion during the Rotary Catalytic Cycle of F1-ATPase. Biophysical Society 60th Annual Meeting, February 2016; Los Angeles, CA, USA; *Biophys. J.* 110(3):312a.

6. M. Kogut, C. Kleist, **J. Czub**. Molecular basis of the stability of G-quadruplexes with human telomeric sequence – molecular dynamics simulations study. The 31st Winter School in Theoretical Chemistry Computational Biochemistry, Helsinki, December 2015, Nr. 13

7. L. Nierzwicki, **J. Czub**. Specific interaction of Amyloid Precursor Protein with Cholesterol: Structure of the Complex and Driving Forces Characterized with Molecular Detail. The 31st Winter School in Theoretical Chemistry Computational Biochemistry, Helsinki, December 2015, Nr. 17

8. B. Adamczak, M. Wieczor, J. Stangret, **J. Czub**. How does betaine stabilize the folded state of proteins?, 58 Zjazd Naukowy Polskiego Towarzystwa Chemicznego w Gdansku, September 2015, Gdansk

9. M. Wieczor, P. Gdaniec and **J. Czub**. The sliding of TRF1 along a helical path on telomeric DNA. 10th European Biophysics Congress, July 2015, Dresden, Germany, P384

10. B. Adamczak, M. Wieczor, M. Kogut, J. Stangret and **J. Czub**. The origin of the effect of osmolytes on protein stability. 10th European Biophysics Congress, July 2015, Dresden, Germany, P617

11. M. Kogut and **J. Czub**. Molecular basis of the stability of human telomeric G-quadruplexes - molecular dynamics simulation study. From Computational Biophysics to Systems Biology (CBSB14), May 2014, Gdansk, Poland, P50

12. M. Wieczor, P. Wityk, A. Tobiszewski and **J. Czub**. Molecular Recognition in Complexes of TRF1/TRF2 Proteins with Telomeric DNA. From Computational Biophysics to Systems Biology (CBSB14) , May 2014, Gdansk, Poland, P51

13. **J. Czub**, M. Wieczor, P. Wityk and H. Grubmueller. Accumulation and transmission of energy during the rotary catalytic cycle of F_1-ATPase. 3rd Annual CCP-BioSim Conference: Frontiers of Biomolecular Simulation, May 2014, Edinburgh, UK, Poster—A8

14. M. Kogut, **J. Czub**. Molecular basis of the stability of G-quadruplexes - molecular dynamics simulation study. 3rd Annual CCP-BioSim Conference: Frontiers of Biomolecular Simulation, May 2014, Edinburgh, UK, Poster—A21

15. Milosz Wieczor, Pawel Wityk, Adrian Tobiszewski and **J. Czub** A Molecular Dynamics study of mechanisms of sequence recognition and DNA binding in two telomeric proteins, TRF1 and TRF2.3rd Annual CCP-BioSim Conference: Frontiers of Biomolecular Simulation, May 2014, Edinburgh, UK, Poster—B46

16. **J. Czub**, M. Wieczor, A. Tobiszewski and H. Grubmueller. Rotation Triggers Nucleotide-Independent Conformational Transition of the Empty Beta Subunit of F1-ATPase. Biophysical Society 58th Annual Meeting, February 2014; San Francisco, CA, USA; *Biophys. J.* 106 (2), 253a

17. Milosz Wieczor, Pawel Wityk, Adrian Tobiszewski and **J. Czub**. Mechanisms of Trf1/Trf2 Binding Properties and DNA Sequence Recognition as Studied by Molecular Dynamics. Biophysical Society 58th Annual Meeting, February 2014; San Francisco, CA, USA; *Biophys. J.* 106 (2), 697a

18. S. Samaritani, M. Baginski, L. Calucci, V. Censi, **J. Czub**, L. Nierzwicki, M. Wieczor, C. Forte. Novel platinum compounds with potential for cancer therapy: study of their interaction with model lipid membranes. 35th FGMR Discussion Meeting & Joint Conference of the German, Italian and Slovenian Magnetic Resonance Societies, September 2013, Frauenchiemsee, Germany, Book of abstracts: P71

19. M. Wieczor, A. Tobiszewski, P. Wityk and **J. Czub**. A molecular Dynamics study of sequence specificity and DNA Winding mechanisms of human telomere recognition factors: TRF1 and TRF2. Polish Biochemical Society Meeting, September 2013, Toruń, Poland, *Acta Biochim. Pol.* (2013) 60 Suppl-1, p. 72, P.4.7

20. L. Nierzwicki and **J. Czub**. Specific interactions between the amyloid precursor and cholesterol in a lipid bilayer by means of moleecular dynamics simulations. Polish Biochemical Society Meeting, September 2013, Toruń, Poland, *Acta Biochim. Pol.* (2013) 60 Suppl-1, p. 49, P.3.23

21. M. Wieczor, A. Tobiszewski, P. Wityk and **J. Czub**. Mechanism of TRF1/TRF2 binding properties and DNA sequence recognition: a molecular dynamics study. 9th European Biophysics Congress, July 2013, Lisbon, Portugal, *Eur. Biophys. J.* (2013) Suppl-1 S137, P-394

22. A. Tobiszewski, M. Wieczor, P. Wityk and **J. Czub**. Interaction of a triazoloacridone derivative C1305 with telomeric DNA through molecular dynamics. 9th European Biophysics Congress, July 2013, Lisbon, Portugal, *Eur. Biophys. J.* (2013) Suppl-1 S137, P-392

23. M. Kogut, M. Wieczor, A. Tobiszewski and **J. Czub**. Molecular basis of the stability of G-quadruplexes – a molecular dynamics simulation study. 9th European Biophysics Congress, July 2013, Lisbon, Portugal, *Eur. Biophys. J.* (2013) Suppl-1 S91, P-215

24. M. Wieczor, A. Tobiszewski, P. Wityk and **J. Czub**. Molecular Recognition in Complexes of Telomeric DNA with TRF Proteins as Studied by Molecular Dynamics Simulations, Biophysical Society 57th Annual Meeting, February 2013; Philadelphia, PA, USA; *Biophys. J.* 104 (2), 255a

25. A. Neumann, M. Baginski and **J. Czub**. Exploring Amphotericin B-Membrane Interactions: Free Energy Simulations; Biophysical Society 57th Annual Meeting, February 2013; Philadelphia, PA, USA; *Biophys. J.* 104 (2), 250a

26. C. Kutzner, **J. Czub** and H. Grubmüller. Driving Macromolecular Rotary Motions in Atomistic Simulations with GROMACS Annual Meeting of German Biophysical Society, September 2012, Goettingen, Germany.

27. A. Neumann, **J. Czub** and M. Baginski. New Insights into the Membrane Mechanism of Action of Amphotericin B from Molecular Dynamics Simulations. Biophysical Society 56th Annual Meeting, February 2012; San Diego, CA, USA; 482-Pos

28. C. Kutzner, **J. Czub** and H. Grubmüller. Keep it flexible: driving macromolecular rotary motion in atomistic simulations with GROMACS. Biophysical Society 56th Annual Meeting, February 2012; San Diego, CA, USA; 848-Pos

29. **J. Czub**. Mechanism of energy transmission in F_1-ATPase as revealed by molecular dynamics simulations. 11th Workshop on Computer Simulation and Theory of Macromolecules April 2011, Hünfeld, Germany

30. A. Neumann, M. Baginski and **J. Czub**. Amphotericin B exhibits qualitatively different affinity for erosterol and for cholesterol in lipid membranes 11th Workshop on Computer Simulation and Theory of Macromolecules, April 2011, Hünfeld, Germany

31. A. Neumann, M. Baginski and **J. Czub**. How do sterols determine the antifungal effect of amphotericin B? Free energy of binding between the drug and its membrane targets. Biophysical Society 55th Annual Meeting, March 2011; Baltimore, MD, USA; 852-Pos

32. **J. Czub** and H. Grubmüller. Microscopic picture of the mechanism of energy transmission in F_1-ATPase as revealed by molecular dynamics simulations. Biophysical Society 55th Annual Meeting, March 2011; Baltimore, MD, USA; 2898-Pos

33. C. Kutzner, **J. Czub** and H. Grubmüller. Studying rotary motions in proteins with GROMACS. 10th Workshop on Computer Simulation and Theory of Macromolecules April 2010, Hünfeld, Germany

34. **J. Czub** and H. Grubmüller. Molecular dynamics studies of the mechanism of energy transduction in F_1-ATPase 10th Workshop on Computer Simulation and Theory of Macromolecules April 2010, Hünfeld, Germany

35. A. Neumann, **J. Czub** and M. Baginski. Mechanism of amphotericin B selective toxicity as suggested by free energy molecular dynamics simulations, 10th Workshop on Computer Simulation and Theory of Macromolecules, April 2010, Hünfeld, Germany

36. **J. Czub** and H. Grubmüller. Spatial distribution of elasticity in the F_1 motor of ATP synthase reveals the microscopic nature of the coupling between the central shaft and the catalytic subunit. Biophysical Society 54th Annual Meeting, February 2010; San Francisco, CA, USA; 869-Pos

37. B. Tomiczek, J. Bidzinska, K. Dzedzej, **J. Czub**, A. Skladanowski and M. Baginski. Molecular properties of telomeric TRF1/TRF2–DNA systems. Biophysical Society 54th Annual Meeting, February 2010; San Francisco, CA, USA; 1393-Pos

38. A. Neumann, **J. Czub** and M. Baginski. On the possibility of the amphotericin B-sterol complex formation in cholesterol- and ergosterol-containing lipid bilayers – a molecular dynamics study. Vienna Summer School Drug Design, September 2009, Vienna, Austria

39. **J. Czub** and H. Grubmüller. Elastic properties of F_1-ATPase as studied by molecular dynamics simulations, 9th Workshop on Computer Simulation and Theory of Macromolecules April 2009, Hünfeld, Germany

40. M. Wojciechowski, **J. Czub**, M. Baginski. Molecular electrostatic properties of human telomeric proteins TRF1 and TRF2. Biophysical Society 52nd Annual Meeting and 16th IUPAB International Biophysics Congress, February 2008; Long Beach, CA, USA; 2020-Pos

41. M. Slisz, B. Cybulska, J. Grzybowska, **J. Czub**, R. Prasad, E. Borowski. Amphotericin B and its nontoxic derivative - MFAmE overcome MDR of fungi by not being substrates of efflux pumps. The 6th AFMC International Medicinal Chemistry Symposium (AIMECS 07), July 2007, Istanbul, Turkey; PC-1

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