Tamás Beke-Somfai

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Scopus Author ID: 35323780200

- **EDUCATION**

09/2007 PhD (*Summa cum laude*, 100%) in Chemistry, Eötvös University, Hungary
06/2001 MSc. in Chemistry, Eötvös University, Hungary

- **CURRENT POSITION**

2015– Group Leader, Biomolecular Self-Assembly "Momentum" Group
Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences

- **PREVIOUS POSITIONS / EMPLOYMENT HISTORY**

2010–2014 Guest Researcher
Dept. of Chemical and Biological Engineering, CHALMERS Univ. of Technology, Sweden
2008–2010 Post Doctoral Fellow
Dept. of Chemical and Biological Engineering, CHALMERS, Sweden
2007–2008 Research Associate
Protein Modeling Group, Hungarian Academy of Sciences, Hungary
2005–2007 Research Assistant
Dept. of Organic Chemistry, Eötvös University, Hungary

- **SCHOLARSHIPS / AWARDED FELLOWSHIPS / DISTINCTIONS**

2018 Nivo prize of the Hungarian Chemical Society
2015-2017 Marie Sklodowska Curie Individual Fellowship
2006 Research scholarship, Gedeon Richter Pharmaceuticals, Hungary
2005 Visiting fellowship, HPC-Europa, CINECA, Italy
2005 Scholarship awarded, Hungarian Peptide and Protein Research Foundation
2004 Kajtár Márton Fund, Fellowship, Hungary

- **AWARDED RESEARCH FUNDS**

2016 PolymEV, National RDI Office, 4 partner consortium grant, 42 months period
Role: Consortium Coordinator, PI
Total budget of the project: ~2.8M EUR, to RCNS: ~904k EUR

2016 Momentum Excellence Grant, PI, ~700k EUR
5 year period, Hungarian Academy of Sciences

2016 Bioinspired Self-Assembly, GINOP Consortial Research Fund, Sub-project, PI
57 months period, ~83k EUR

2015 Internal Collaboration Grant, Inst. Mat.and Env. Chem., PI, ~17k EUR
Internal Grant of the Research Centre for Natural Sciences

2014 Elite Nanyang Assistant Professorship (NAP), PI, ~800k USD
Internal Grant of Nanyang Technological University (NTU), Singapore,
Overall package included funding of 4 PhD students, additional 800k USD research grant, distinguished salary and benefits for PI. Awarded, but not taken (parental leave)

2013 Young investigator research grant, PI, ~72.5k EUR
3 year period, Hungarian Scientific Research Fund

2011 Basic research grant, Co-applicant, ~630k / ~250k EUR)
4 year period, Swedish Research Council, to coapplicant Beke-Somfai: 250kEUR
(PI: Prof. Bengt Nordén)

2008 Young investigator research grant, PI, ~16.5k EUR
Hungarian Scientific Research Fund
Awarded but not taken, post-doc offer at CHALMERS accepted before decision

- **ACADEMIC EXPERIENCE / VISITING FELLOWSHIPS**

2008 University of San Luis, Argentina, Visiting Research Fellow (1 month)
2005 University of Bologna, CINECA Centre, Italy, Visiting Fellow (4 months)
2004 University of Shanghai, China, Junior Visitor (1 month)
2002–2003 University of Debrecen, Hungary Visiting Fellow (6 months)

- **TEACHING ACTIVITIES / ORGANIZED CONFERENCES**

2017 "Molecular Frontiers, Budapest", Main organizer, Symposium on Proteins and Medicine, 4 Nobel laurate speakers, 1000+ participants, broadcasted on national TVs and radios, reaching 100 000+ people on social media.

2015– "World of Molecules" Lecturing organic chemistry of biomolecules for first year undergraduate students at Peter Pázmány Catholic University, Budapest

2009–2012 Teoretisk Kemi (Theoretical Chemistry) – Assistant, CHALMERS, Sweden

2007–2008 Lecturing "Practical Theoretical Organic Chemistry" Special college in English for MSc students, Eötvös University, Hungary

- **REVIEWER ACTIVITIES**

Grant applications:

2020 Czech Academy of Sciences, 5yr evaluation of Institute Groups, *ad hoc* reviewer
2018– Natural Science Advisory Board, Hungarian Academy of Sciences, Board member
2016–2019 Hungarian Research Fund, Board member, Medical Chemistry
2010– Unity Through Knowledge Fund, Croatia, *ad hoc* reviewer
2008– Hungarian Research Fund, *ad hoc* reviewer

Referee for scientific journals:

Langmuir; J. Am. Chem. Soc.; Quart. Rev. Biophys; BBA-Proteins and Proteomics; J. Phys. Chem.; J. Mol. Graph. and Modelling; Curr. Org. Chem.; Phys. Biol.; Math. Biosci.; Coll. & Surf. B; J. Funct. Biomat., Small, RSC Chem. Biol., Advanced Science,

- **SCIENTOMETRIC DATA**

Number of scientific papers: 65 (52 Q1, 29 D1)
Number of citations (Google Scholar): 1000
H-index: 17
Aggregated impact factor: 350

- **OUTREACH ACTIVITIES**

2009– Volunteer at Molecular Frontiers Foundation (*www.molecularfrontiers.org)*
2009– Special Advisor at Neocore Games
Interactive entertainment products development (www.neocoregames.com)
"King Arthur: The Roleplaying Wargame"
2004–2005 Scientific Advisor: "Preparing for graduation: Chemistry"
TV Series, National TV (M2), www.asta.hu

1997– Translator at HUNGALIBRI Publisher
English to Hungarian, "Windows 95 for Dummies", published in 1997.

- **LANGUAGE PROFICIENCY**

English: Fluent (Advanced State Exam 1996)
Swedish: Very good command
German, Italian: Basic (German Basic State Exam 2005)
Hungarian: Native

- **FAMILY STATUS**

Married, 4 children, Ráhel (2009), Máté (2010), Csenge (2012) and Erik (2016)

- **CAREER BREAKS IN RESEARCH**

11/2013–02/2015 Parental leave

Full List of Publications

1) A. Wacha, **T. Beke-Somfai**: PmlBeta: A PyMOL extension for building beta-amino acid insertions and beta-peptide sequences, *SoftwareX*, **2021**, *13*, 100654

   IF: 2.14

2) B. Balogh, M. Ivánczi, B. Nizami, **T. Beke-Somfai**, I. Mándity: ConjuPepDB: a database of peptide-drug conjugates, *Nucl. Acid. Res.*, **2021**, *D1*, D1094-D1101

   IF: 11.147

3) M. Quemé-Pena, M. Ricci, T. Juhász, K. Horváti, Sz. Bősze, B. Biri-Kovács, B. Szeder, F. Zsila, **T. Beke-Somfai***: Old Polyanionic Drug Suramin Suppresses Detrimental Cytotoxicity of the Host Defense Peptide LL-37, *ACS Pharma. Transl. Sci.*, doi: 10.1021/acsptsci.0c00155

   IF: N/A

4) Y. Xiao, S. Rocha, C. C. Kitts, A. Reymer, **T. Beke-Somfai**, K. Frederick, B. Nordén: Michler's Hydrol Blue Elucidates Structural Differences in Prion Strains, *Proc. Natl. Acad. Sci.*, **2020**, *117*, 29677-29683

   IF: 9.412

5) P.Singh, I. Cs. Szigyártó, M. Ricci, F. Zsila, T. Juhász, J. Mihály, Sz. Bősze, J. Kardos, D. Kitka, Z. Varga, **T. Beke-Somfai***: Membrane active peptides remove surface adsorbed protein corona from extracellular vesicles of red blood cells, *Frontiers in Chemistry*, **2020**, *8* : 703, doi: 10.3389/fchem.2020.00703

   IF: 3.693

6) I. Cs. Szigyártó, J. Mihály, A. Wacha, D. Bogdán, T. Juhász, G. Kohut, G. Schlosser, F. Zsila, V. Urlacher, Z. Varga, F. Fülöp, A. Bóta, I. Mándity, **T. Beke-Somfai***: Membrane active Janus-oligomers of β^3-peptides, *Chemical Science*, **2020**, *11*, 6868-6881

   IF: 9.346

7) F. Zsila, **T. Beke-Somfai**: Human host-defense peptide LL-37 targets stealth siderophores, *Biochem. Biophys. Res. Commun.* **2020**, *526*, 780-785

   IF: 2.705

8) A. Said-Ståhlsmeden, A. J. Paterson, I. Cs. Szigyártó, L. Thunberg, J. R. Johansson, **T. Beke-Somfai***, N. Kann: Chiral 1,5-disubstituted 1,2,3-triazoles - versatile tools for foldamers and peptidomimetic applications, *Organic & Biomolecular Chemistry*, **2020**, *18*, 1957-1967

   IF: 3.490

9) M. Ricci, K. Horváti, T. Juhász, I. Szigyártó, Gy. Török, F. Sebák, A. Bodor, L. Homolya, J. Henczkó, B. Pályi, T. Mlinkó, J. Mihály, B. Nizami, Z. Yang, F. Lin, X. Lu, L. Románszki, A. Bóta, Z. Varga, Sz. Bősze, F. Zsila, **T. Beke-Somfai***: Anionic Food Color Tartrazine Enhances Antibacterial Efficacy of Histatin-derived Peptide DHVAR4 by Fine-Tuning its

Membrane Activity *Quarterly Reviews of Biophysics*, **2020**, *53*, E5, DOI: 10.1017/S0033583520000013

IF: 6.643

10) C. Wang, Y. Luo, X. Li, F. Zhang, F. Wang, X. Han, T. Wang, **T. Beke-Somfai**, X. Lu: Revealing Molecular-Level Interaction between a Polymeric Drug and Model Membrane via SFG and Microfluidics, *Langmuir*, **2020**, *36*, 1615-1622

IF: 3.683

11) R. Deák, J. Mihály, I. Cs. Szigyártó, **T. Beke-Somfai**, L. Turiák, L. Drahos, A. Wacha, A. Bóta, Z. Varga: Nanoerythrosomes tailoring: Lipid induced protein scaffolding in ghost membrane derived vesicles *Materials Science & Engineering C,* **2020**, *109,* 110428

IF: 5.880

12) B. Nizami, D. Bereczki-Szakál, N. Varró, K. Battioui, V. U. Nagaraj, I. Szigyártó, I. Mándity, **T. Beke-Somfai***: FoldamerDB: A database of peptidic foldamers *Nucl. Acid. Res.* **2020,** *D1, D1122-D1128*

IF: 11.147

13) F. Zsila, Sz. Bősze, **T. Beke-Somfai**: Interaction of antitubercular drug candidates with α1-acid glycoprotein produced in pulmonary granulomas *Int. J. Biol. Macromol.* **2020**, *147*, 1318-1327

IF: 3.909

14) D. Kitka, J. Mihály, J-L Fraikin, **T. Beke-Somfai**, Z. Varga: Detection and phenotyping of extracellular vesicles by size exclusion chromatography coupled with on-line fluorescence detection *Scientific Reports*, **2019**, *9, 1,* 19868

IF: 4.011

15) F. Wang, X. Li, F. Zhang, X. Liu, P. Hu, **T. Beke-Somfai**, X. Lu: Revealing Interfacial Lipid Hydrolysis Catalyzed by Phospholipase A_1 at Molecular Level via Sum Frequency Generation Vibrational Spectroscopy and Fluorescence Microscopy, *Langmuir*, **2019**, *35*, 12831-12838

IF: 3.683

16) A. Wacha, **T. Beke-Somfai***, T. Nagy Improved Modeling of Peptidic Foldamers Using a Quantum Chemical Parametrization Based on Torsional Minimum Energy Path Matching, *ChemPlusChem*, **2019**, *84*, 927-941

Invited article IF: 3.4413

17) G. Kohut, A. Sieradzan, F. Zsila, T. Juhász, Sz. Bősze, A. Liwo, S. Samsonov, **T. Beke-Somfai***: The molecular mechanism of structural changes in the antimicrobial peptide CM15 upon complex formation with drug molecul suramin: a computational analysis *Phys. Chem. Chem. Phys.* **2019**, *21*, 10644-10659

IF: 3.906

18) F. Zsila, G. Kohut, **T. Beke-Somfai***: Disorder-to-helix conformational conversion of the human immunomodulatory peptide LL-37 induced by antiinflammatory drugs, food dyes and some metabolites, *Int. J. Biol. Macromol.* **2019**, *129*, 50-60.

IF: 3.909

19) M. Quemé-Pena, T. Juhász, J. Mihály, I. Cs. Szigyártó, K. Horváti, Sz. Bősze, J. Henczkó, B. Pályi, Cs. Németh, Z. Varga, F. Zsila, **T. Beke-Somfai***: Manipulating Active Structure and Function of Cationic Antimicrobial Peptide CM15 by the Polysulfonated Drug Suramin: A Step Closer to *in vivo* Complexity *ChemBioChem*, **2019**, *20*, 1578-1590

Invited article IF: 2.774

20) T. Juhász, J. Mihály, G. Kohut, C. Németh, K. Liliom, **T. Beke-Somfai***: The lipid mediator lysophosphatidic acid induces folding of disordered peptides with basic amphipathic character into rare conformations *Scientific Reports*, **2018**, *8*, 14499

IF: 4.122

21) G. Kohut, A. Liwo, S. Bosze, **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

IF: 3.177

22) U. Uciechowska-Kaczmarzyk, S. Babik, F. Zsila, K. K. Bojarski, **T. Beke-Somfai**, S. A. Samsonov: Molecular Dynamics-based model for VEGF-A and its heparin interactions *J. Mol. Graph. Model.*, **2018**, *82*, 157-166

IF: 1.885

23) F. Zsila, T. Juhász, G. Kohut, and **T. Beke-Somfai***: Heparin and Heparan Sulfate Binding of the Antiparasitic Drug 2 Imidocarb: Circular Dichroism Spectroscopy, Isothermal Calorimetry, 3 and Computational Studies, *J. Phys. Chem. B* **2018**, *122*, 1781-1791

IF: 3.177

24) I. Cs. Szigyártó, R. Deák, J. Mihály, S. Rocha, F. Zsila, Z. Varga, **T. Beke-Somfai***: Flow-Alignment of Extracellular Vesicles: Structure and Orientation of Membrane Associated Biomacromolecules Studied with Polarized Light, *ChemBioChem*, **2018**, *19*, 545-551

IF: 2.847

25) F. Zsila, T. Juhász, Sz. Bősze, K. Horváti, I. Cs. Szigyártó, **T. Beke-Somfai***: Hemin and bile pigments are the secondary structure regulators of intrinsically disordered antimicrobial peptides *Chirality*, **2018**, *30*, 195-205

IF: 1.956

26) R. Kiss, M. Zhu, B. Jójárt, A. Czajlik, K. Solti, Balázs Fórizs, É. Nagy, F. Zsila, **T. Beke-Somfai**, G. Tóth: Structural Features uf human DJ-1 in distinct Cys106 oxidative states and their relevance to its loss of function in disease *BBA – General subjects*, 2017, *1861*, 2619-2629

IF: 4.702

27) F. Zsila, Sz. Bősze, K. Horváti, I. Cs. Szigyártó, **T. Beke-Somfai***: Drug and dye binding

induced folding of the intrinsically disordered antimicrobial peptide CM15, *RSC Advances*, 2017, *7*, 41091-41097

IF: 3.108

28) N. Bosaeus, A. Reymer, **T. Beke-Somfai**, T. Brown, M. Takahashi, P. Wittung-Stafshede, S. Rocha, B. Nordén: A stretched conformation of DNA with a biological role?, *Quarterly Reviews of Biophysics*, 2017, *50*, 1-11

IF: 5.627

29) J. Mihály, R. Deák, I. Cs. Szigyártó, A. Bóta, **T. Beke-Somfai**, Z. Varga: Characterization of extracellular vesicles by IR spectroscopy: Fast and simple classification based on amide and C-H stretching vibrations, *Biochim. Biophys. Acta – Biomembranes*, 2017, *1859*, 459-466

IF: 2.847

30) J. Johansson, **T. Beke-Somfai***, A. Said Stalsmeden, N. Kann: Ruthenium-Catalyzed Azide Alkyne Cycloaddition Reaction: Scope, Mechanism and Applications, *Chemical Reviews*, 2016, *116*, 14726-14768

IF: 47.928

31) S. Rocha, M. Kogan, **T. Beke-Somfai**, B. Nordén: Probing Microscopic Orientation in Membranes by Linear Dichroism, *Langmuir*, 2016, *32*, 2841-2846

IF: 3.993

32) F. Zsila, **T. Beke-Somfai**: Dimeric Binding of Plant Alkaloid Ellipticine to Human Serum Proteins, *RSC Advances*, 2016, *6*, 44096

IF: 3.289

33) A. Reymer, S. Babik, M. Takahashi B. Nordén, **T. Beke-Somfai***: ATP Hydrolysis in the RecA–DNA Filament Promotes Structural Changes at the Protein–DNA Interface *Biochemistry*, 2015, 54 (30), pp 4579–4582

IF: 3.015

34) N. Kann, J. R. Johansson, **T. Beke-Somfai***: Conformational properties of 1,4- and 1,5-substituted 1,2,3-triazole amino acids – building units for peptidic foldamers, *Organic & Biomolecular Chemistry*, 2015, *13*, 2776-2785

IF: 3.487

35) A. Reymer, Frederick, K., S. Rocha, **T. Beke-Somfai**, C. C. Kitts, S. Lindquist, B. Nordén: Orientation of aromatic residues in amyloid cores: Structural insights into prion fiber diversity *Proc. Natl. Acad. Sci., U.S.A.*, 2014, *111*, 17158-17163

IF: 9.737

36) L.H. Fornander, B. Feng, **T. Beke-Somfai**, B. Nordén: UV Transition Moments of Tyrosine, *J. Phys. Chem. B*, 2014, *118*, 9247-9257

IF: 3.607

37) M. Kogan, B. Feng, B. Nordén, S. Rocha, **T. Beke-Somfai***: Shear-Induced Membrane

Fusion in Viscous Solutions *Langmuir,* 2014, *30*, 4875-4878

IF: 4.187

38) J. Johansson, E. Hermansson, N. Kann, B. Nordén, **T. Beke-Somfai***: δ-Peptides from RuAAC-Derived 1,5-Disubstituted Triazole Units, *Eur. J. Org. Chem.* 2014, *13*, 2703-2713

IF: 3.443

39) M. Hammarson, J.R. Nilsson, S. Li, **T. Beke-Somfai**, J. Andréasson: Characterization of the Thermal and Photoinduced Reactions of Photochromic Spiropyrans in Aqueous Solution, *J. Phys. Chem. B*, 2013, *117*, 13561-13571

IF: 3.607

40) M. Kogan, B. Nordén, **T. Beke-Somfai***: High Anisotropy of Flow-aligned Bicellar Membrane Systems, *Chemistry and Physics of Lipids,* 2013, *175*, 105-115

IF: 2.147

41) F. Jonsson, **T. Beke-Somfai**, J. Andréasson, B. Nordén: Interactions of a Photochromic Spiropyran with Liposome Model Membranes *Langmuir*, 2013, *29*, 2099-2013

IF: 4.187

42) **T. Beke-Somfai***, P. Lincoln, B. Nordén: Rate of hydrolysis in ATP synthase is fine-tuned by α-subunit motif controlling active site conformation *Proc. Natl. Acad. Sci., U.S.A.*, 2013, *110*, 2117-2122

IF: 9.737

43) **T. Beke-Somfai**, B. Feng, B. Nordén: Energy Phase Shift as Mechanism for Catalysis, *Chem. Phys. Lett.*, 2012, *535*, 169-172

IF: 2.145

44) M. Matson, N. Carlsson, **T. Beke-Somfai**, B. Nordén: Spectral Properties and Orientation of Voltage-Sensitive Dyes in Lipid Membranes, *Langmuir*, 2012, *28*, 10808-10817

IF: 4.187

45) G. Pohl, **T. Beke-Somfai**, I. G. Csizmadia, A. Perczel: Exploiting diverse stereochemistry of β-amino acids: toward a rational design of sheet-forming β-peptide systems *Amino Acids*, 2012, *43*, 735-749

Invited article IF: 3.914

46) M. Kogan, **T. Beke-Somfai***, B. Nordén,: Flow-alignment of bicellar lipid mixtures: orientations of probe molecules and membrane-associated biomacromolecules in lipid membranes studied with polarized light *Chem. Commun.*, 2011, *47*, 7356-7358

IF: 6.378

47) C. C. Kitts, **T. Beke-Somfai**, B. Nordén: Michler's Hydrol Blue: A Sensitive Probe for Amyloid Fibril Detection *Biochemistry*, 2011, *50*, 3451-3461

Highlighted by Editorial Board IF: 3.377

48) **T. Beke-Somfai***, P. Lincoln, B. Nordén: Double-lock ratchet mechanism revealing the role

of αSER-344 in F_oF_1 ATP synthase *Proc. Natl. Acad. Sci., U.S.A.,* 2011, *108*, 4828-4833

IF: 9.737

49) V. Harmat, K. Domokos, D. K. Menyhárd, A. Palló, Z. Szeltner, I. Szamosi, **T. Beke-Somfai**, G. Náray-Szabó, L. Polgár: Structure and Catalysis of Acylaminoacyl Peptidase: Closed and Open Subunits of a Dimer Oligopeptidase *J. Biol. Chem.*, 2011, *286*, 1987-1998

IF: 4.651

50) **T. Beke-Somfai***, P. Lincoln, B. Nordén: Mechanical Control of ATP Synthase Function: Activation Energy Difference between Tight and Loose Binding Sites *Biochemistry*, 2010, *49*, 401-403

IF: 3.377

51) G. Pohl, **T. Beke**, I. G. Csizmadia, A. Perczel: Extended Apolar β-Peptide Foldamers: The Role of Axis Chirality on β-Peptide Sheet Stability *J. Phys. Chem. B*, 2010, *114*, 9338–9348

IF: 3.607

52) **T. Beke-Somfai***, A. Perczel: Zipper-Like Unfolding of β-Sheets Accessed by Pioneer Water Molecules: Atomic Resolution of Forced Unfold Reveals Different Mechanisms for Parallel and Antiparallel Motifs *J. Phys. Chem. Lett.*, 2010, *1*, 1341-1345

IF: 6.585

53) **T. Beke**, Cs. Somlai, G. Magyarfalvi, A. Perczel, Gy. Tarczay: Chiral and Achiral Fundamental Conformational Building Units of β-Peptides: Isolation Conformational Study on Ac-β-HGly-NHMe and Ac-β-HAla-NHMe *J. Phys. Chem. B*, 2009, *113*, 7918-7926

IF: 3.607

54) K. E. Kövér, **T. Beke**, A. Lipták, A. Perczel: OH-rotamer equilibrium of polyalcohols determined by combined NMR three-bond scalar coupling measurements and QM calculations *J. Comput. Chem.* 2009, *30*, 540-550

IF: 3.835

55) A. Czajlik, **T. Beke**, A. Bottoni, A. Perczel: Structure and Stability of Short β-Peptide Nanotubes: a Non-Natural Representative of Collagen *J. Phys. Chem. B* 2008, *112*, 7956-7966

IF: 3.607

56) **T. Beke**, A. Czajlik, B. Bálint, A. Perczel: A Theoretical Comparison of Self-Assembling α- and β-Peptide Nanostructures: Toward Design of β-Barrel Frameworks *ACS Nano*, 2008, *2*, 545-553

IF: 12.062

57) A. Palló, Á. Bencsura, L. Héja, **T. Beke**, A. Perczel, J. Kardos, Á. Simon: Major human γ-aminobutyrate transporter: *In Silico* prediction of substrate efficacy *Biochem. Biophys. Res. Comm.* 2007, *364,* 952-958

IF: 2.406

58) I. Berente, **T. Beke**, G. Náray-Szabó: Quantum mechanical studies on the existence of a trigonal bipyramidal phosphorane intermediate in enzymatic phosphate ester hydrolysis *Theor. Chem. Acc.,* 2007, **118** 129-134

Invited article IF: 2.233

59) G. Pohl, **T. Beke**, J. Borbély, A. Perczel: Prediction of folding preference of 10kDa silk-like proteins using a lego-approach and *ab initio* calculations *J. Am. Chem. Soc.,* 2006, *128,* 14548-14559

IF: 10.677

60) **T. Beke**, I. G. Csizmadia, A. Perczel: Theoretical study on tertiary structural elements of β-peptides: Nanotubes formed from parallel-sheet-derived assemblies of β-peptides *J. Am. Chem. Soc.,* 2006, *128,* 5158-5167

IF: 10.677

61) **T. Beke**, C. Somlai, A. Perczel: Toward A Rational Design of β-Peptide Structures *J. Comput. Chem.* 2006, *27*, 20-38

IF: 3.835

62) **T. Beke**, A. Czajlik, I. G. Csizmadia, A. Perczel: Determining suitable *lego*-structures to estimate stability of larger peptide nanostructures using computational methods *Phys. Biol., Special Issue on Nanobiology,* 2006, *3* S26-S39

Invited article IF: 2.620

63) **T. Beke**, I. G. Csizmadia, A. Perczel: On the flexibility of β-peptides *J. Comput. Chem.,* 2004, *25*, 285-307.

IF: 3.835

64) A. Láng, A. K. Füzéry, **T. Beke**, P. Hudáky, A. Perczel: Potential Energy Curves, Surfaces and Hypersurfaces. A model to follow and understand the conformational transformations in amino acids *J. Mol. Struct., Special Issue* 2004, *675*, 163-175

Invited article IF: 1.371

65) P. Hudáky, **T. Beke**, A. Perczel: Side-chain conformational potential energy surfaces associated with all major backbone folds of neutral tautomers of N- and C-protected L-histidine *J. Mol. Struct.* 2002, *583,* 117-135

IF: 1.371

Book Chapters / Popular Scientific Articles

T. Beke-Somfai Speed Evolution – Felgyorsított Evolúció: A 2018-as Kémiai Nobel díj *Hungarian Periodicals, 2019, 180, 9, 1386-1389,* DOI: 10.1556/2065.180.2019.9.13

T. Beke, A. Perczel: The Thermodynamic Driving Force of Sheet Structures. Formation and Stability Conditions of Nanotubes *BIOforum Europe*, **2008,** *5*, 038-041 (*Invited contribution*)

T. Beke, M. A. Sahai, M. Stenta, A. Perczel, A. Bottoni, I. G. Csizmadia: A DFT Computational Investigation of the Catalytic Mechanism of Glutathione Peroxidase *HPC-Europa, Science and Supercomputing in Europe/Chemistry*, **2005**, pp. 46-54, ISBN 88-86037-17-1 (*Invited contribution*)

Invited Oral Seminars at International Symposia

1. *June 2006, TAM Meeting-HPC Europa, Barcelona, Spain,* "A DFT Computational Investigation of the Catalytic Mechanism of Gluthation Peroxidase"
2. *June 2010, 35th FEBS Congress, Gothenburg, Sweden* "The reaction mechanism in ATP synthase: mechanical control by structural changes in the active sites"
3. *September, 2010, Zaragoza, Spain* Invited Participant on the workshop "Peptide Databases in Quantum Chemistry"
4. *September 2011, 4th ECCLS, Budapest, Hungary* "A Quantum Mechanical Study on the Reaction Mechanism in ATP Synthase"
5. *April 2012, BIT's 3rd Symposium, Xi'an, China* "Double-Ratchet Mechanism in FoF1 ATP Synthase. Potential Applications Using Computer-aided Design"
6. *September 2012, SUPRA Meeting, Marstrand, Sweden* "Combining light spectroscopy data with theoretical calculations for improved molecular interpretation"
7. *October 2013, Chalmers, Presenting of the Nobel Laurates in Chemistry 2013, Gothenburg* "And the winners are…"

Oral Presentation at International Symposia

May, 2007, Centenary Conference of the Hungarian Chemical Society, Sopron, Hungary
„From Amino acids to Nanotubes: Theoretical Investigation of β-Peptide Nanotubes" (Oral presentation)

June, 2013, 5th European Conference on Chemistry for Life Sciences, Barcelona, Spain
"ATP Synthase: The Complex Biomolecular Machine" (Extended Oral Presentation)

September, 2013,9th European Conference on Computational Chemistry, Sopron, Hungary
"Hyperfine Tuning in Complex Biomolecular Machines" (Oral presentation)

Peer-Reviewed Conference Contributions

June 2011, 36th FEBS Congress, Torino, Italy,
„Double-lock reaction mechanism in ATP synthase: Mechanical control by structural changes in the active sites" *Febs Journal, 278,* 96, **2011**

March 2011, 241st ACS Meeting, Anaheim, CA

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