

Tamás Beke-Somfai

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- **EDUCATION**

09/2007 PhD (*Summa cum laude*) in Chemistry, Eötvös University, Hungary

06/2001 MSc. In Chemistry, Eötvös University, Hungary

- **CURRENT POSITION**

2023– Vice Director,
Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences

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 (Bengt Nordén group, Chair, Nobel Prize of Chemistry)
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 Skłodowska 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 (LAST 5 YEARS)**

2022 Élvonal – „Frontiers” Excellence Grant, National RDI Office, 60 months, PI, ~900k EUR

2021 “TKP” consortial grant for “Sustainable Agriculture”, Coordinator, PI, to TTK ~870k EUR

2020 “Piaci KFI 2020” Support for Market-driven Research, Development and Innovation

Projects (NRDI), 60 months, Leader: ToxiCOOP Inc, Coordinator of Development at TTK,
Total budget: ~2M EUR, to TTK ~800k EUR.

- 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 TTK: ~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
- 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 laureate speakers, 1000+ participants, broadcasted on national TVs and radios, reaching 100 000+ people on social media.
- 2021– “Bionanotechnology” assembled and lecture the course for MA and PhD level students at Peter Pázmány Catholic University, Budapest
- 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:

2022	Medical Research Council (MRC), United Kingdom (UK-RI), <i>ad hoc</i> reviewer
2022	ANR (National Research Agency), France, <i>ad hoc</i> reviewer
2020	Czech Academy of Sciences, 5yr evaluation of Institute Groups, <i>ad hoc</i> 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, <i>ad hoc</i> reviewer
2008–	Hungarian Research Fund, <i>ad hoc</i> reviewer

Referee for scientific journals:

Advanced Science, Advanced Materials, Journal of Extracellular Vesicles, 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.

• OUTREACH ACTIVITIES

2021–	Member of the Hungarian Young Academy (HYA), working on various projects and organizing to improve statues of young researchers
2015–	Organizing annual workshops on Marie-Curie actions for individual fellows, as part of HYA and in cooperation with the National Research and Development Institute (NRDI - NKFIH)
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

• MEMBERSHIPS

Member of European Chemical Society
Member of International Society of Extracellular Vesicles
Member of Biophysical Society
Member of European Peptide Society
Member of Hungarian Chemical Society
Member of Hungarian Biophysical Society
Member of Hungarian Biochemical Society
Committee Member of the Hungarian Academy of Sciences
Member of the Hungarian Young Academy

Full List of Publications

- 1) C. Bellini, U. Atxabal, S. Bősze, O. Dobay, A. Horváth, I. Cs. Szigyártó, **T. Beke-Somfai**, J. Jiménez-Barbero, I. Puskás, K. Horváti Supramolecular Complexes of Ultrashort Cationic Lipopeptides with Cyclodextrins: Improved Selectivity and Therapeutic Potential *Aggregate*, **2025**, *e741*
IF: 13.9
- 2) I. Cs. Szigyártó, P. Singh, T. Sonallya, L. Románszki, J. Mihály, Z. Wiener, T. Bebesi, G. Mészáros, Z. Keresztes, M. Thompson, Z. Varga, **T. Beke-Somfai*** ATR-Infrared Spectroscopy and Acoustic Sensing in Characterization of Blood and Pancreatic Ductal Adenocarcinoma-Derived Extracellular Vesicles. In: Matta, C., Mobasheri, A., Takács, R. (eds) *The Surfaceome. Methods in Molecular Biology*, vol 2908. Humana, New York, NY. **2025**, 225-238
- 3) T. Sonallya, A. Gaál, I. Cs. Szigyártó, Z. Varga, **T. Beke-Somfai*** Biophysical Profiling of Protein Corona on Red Blood Cell-Derived Extracellular Vesicles (REVs): Linear Dichroism and Microfluidic Resistive Pulse Sensing Separate Surface Clearing from Vesicle Disruption. **2025** 213-223 In: Matta, C., Mobasheri, A., Takács, R. (eds) *The Surfaceome. Methods in Molecular Biology*, vol 2908. Humana, New York
- 4) S. Chakraborty, K. El Battioui, T. Sonallya, I. Cs Szigyártó, Z. Varga, T. Juhász, **T. Beke-Somfai*** Charge and length dependent build-up of environment sensitive lamellin β -peptides *Phys. Chem. Chem. Phys*, **2025**, 27, 8540-8551
IF: 2.9
- 5) T. Sonallya, T. Juhász, I. Cs. Szigyártó, K. Ilyés, P. Singh, D. Khamari, E. I. Buzás, Z. Varga, **T. Beke-Somfai***, Categorizing interaction modes of antimicrobial peptides with extracellular vesicles: Disruption, membrane trespassing, and clearance of the protein corona *J. Coll. & Int. Sci.* **2025**, 679, 496-509
IF: 9.4
- 6) O. Pavela, T. Juhász*, L. Tóth, A. Czajlik, Gy. Batta, L. Galgóczy*, **T. Beke-Somfai*** : Mapping of the Lipid-Binding Regions of the Antifungal Protein NFAP2 by Exploiting Model Membrane *J. Chem. Inf. Model.* **2024**, 64, 16, 6557–6569
IF: 5.6
- 7) F. Ferrara, **T. Beke-Somfai**, N. Kann*: Recent Developments in the Ruthenium-Catalyzed Azide Alkyne Cycloaddition (RuAAC) Reaction, *EurJOC*, **2024**, 10.1002/ejoc.202400113
IF: 2.8
- 8) K. El Battioui, S. Chakraborty, A. Wacha, D. Molnár, M. Quemé-Peña, I. Cs. Szigyártó, Cs. L. Szabó, A. Bodor, K. Horváti, G. Gyulai, Sz. Bősze, J. Mihály, B. Jezsó, L. Románszki, J. Tóth, Z. Varga, I. Mándity, T. Juhász, **T. Beke-Somfai***: In situ captured antibacterial action of membrane incising peptide lamellae, *Nat. Commun*, **2024**, 15, 3424

IF: 16.6

- 9) Welsh et al.: Minimal Information for studies of extracellular vesicles (MISEV2023): From basic to advanced approaches, *J. Extracell. Ves.*, **2024**, *13*, e12404

IF: 16.0

- 10) S. Chakraborty*, K. El Battoui, **T. Beke-Somfai***: Peptide-based Assemblies for Supercapacitor Applications, *Small Science*, **2024**, *4*, 2300217

IF: 12.7

- 11) E. N. Frigini, R. D. Porasso, **T. Beke-Somfai**, J. J. López Cascales, R. D. Enriz, S. Pantano* The Mechanism of Antimicrobial Small-Cationic Peptides from Coarse-Grained Simulations, *J. Chem Inf. Model*, **2023**, *63*, 21, 6877-6889

IF: 5.6

- 12) T. Juhász, M. Quemé-Peña, **T. Beke-Somfai*** Unique thermophoretic behavior of supramolecular assemblies of cationic antimicrobial peptides with anionic small molecule agents, *J. Mol. Liquids*, **2023**, 122513,

IF: 6

- 13) A. Wacha, Z. Varga, **T. Beke-Somfai***: Comparative Study of Molecular Mechanics Force Fields for beta-Peptidic Foldamers: Folding and Self-Association, *J. Chem Inf. Model*, **2023**, *63*, 12, 3799-3813

IF: 5.6

- 14) P. Singh, I. Cs. Szigyártó, M. Ricci, A. Gaál, M. M. Queme Peña, D. Kitka, L. Fülöp, L. Turiák, L. Drahos, Z. Varga, **T. Beke-Somfai***: Removal and identification of external protein corona members from RBC-derived extracellular vesicles by surface manipulating antimicrobial peptides, *Journal of Extracellular Biology*, **2023**, DOI: 10.1002/jex2.78

IF: N/A

- 15) V. U. Nagaraj, T. Juhász, M. Quemé-Peña, I. Cs. Szigyártó, D. Bogdán, A. Wacha, J. Mihály, L. Románszki, Z. Varga, J. Andréasson, I. Mándity, **T. Beke-Somfai***: Stimuli-Responsive Membrane Anchor Peptide Nanofoils for Tunable Membrane Association and Lipid Bilayer Fusion, *ACS Appl. Mater. Interfaces*, **2022**, *14*, 55320

IF: 10.383

- 16) Z. Varga, M. Madai, G. Kemenesi, **T. Beke-Somfai**, F. Jakab*: Single-particle detection of native SARS-CoV-2 virions by microfluidic resistive pulse sensing, *Colloids and Surfaces B: Biointerfaces* **2022**, *218*, 112716

IF: 5.79

- 17) V. Tóth, H. Vadászi, L. Ravasz, D. Mittli, D. Mátyás, T. Molnár, A. Micsonai, T. Szaniszló, P. Lőrincz, R. Kovács, T. Juhász, **T. Beke-Somfai**, G. Juhász, B. A. Györffy, K. A. Kékesi, J. Kardos*: Neuronal-specific septin-3 binds Atg8/LC3B, accumulates and localizes to autophagosomes during induced autophagy, *Cell. Mol. Life Sci.*, **2022**, *78*, 9, 1-18

IF 9.261

- 18) T. Bebesi, D. Kitka, A. Gaál, I. Cs. Szigyártó, R. Deák, **T. Beke-Somfai**, K. Korpivanacz, T. Juhász, A. Bóta, Z. Varga, J. Mihály: Storage conditions determine the characteristics of red blood cell derived extracellular vesicles, *Scientific Reports*, **2022**, *12*, 977

IF: 4.379

- 19) Paterson, A. J.; **Beke-Somfai, T.**; Kann, N., In *Science of Synthesis: Click Chemistry*, Rutjes, F. P. J. T., Ed.; Thieme: Stuttgart, **2022**; p 289-335. DOI: 10.1055/sos-SD-235-00118

- 20) F. Zsila, M. Ricci, I. Cs. Szigyártó, P. Singh, **T. Beke-Somfai***: Quorum Sensing Pseudomonas Quinolone Signal Forms Chiral Supramolecular Assemblies with the Host Defense Peptide LL-37, *Front. Mol. Biosci.*, **2021**, *8*, 742023

IF: 4.259

- 21) T. Juhász, M. Quemé-Peña, B. Kővágó, J. Mihály, M. Ricci, K. Horváti, Sz. Bősze, F. Zsila, **T. Beke-Somfai***: Interplay between membrane active host defense peptides and heme modulates their assemblies and in vitro activity, *Scientific Reports*, **2021**, *11*, 18328

IF: 4.379

- 22) D. Papp, I.C. Szigyártó, B. Nordén, A. Perczel, **T. Beke-Somfai***: Structural Water Stabilizes Protein Motifs in Liquid Protein Phase: The Folding Mechanism of Short β -Sheets Coupled to Phase Transition, *Int. J. Mol. Sci.*, **2021**, *22*, 8595

IF: 5.923

- 23) M. Quemé-Peña, T. Juhász, G. Kohut, M. Ricci, P. Singh, I. C. Szigyártó, Z. I. Papp, L. Fülöp, **T. Beke-Somfai***, *Int. J. Mol. Sci.*, **2021**, *22*, 8613

IF: 5.923

- 24) B. Lima, M. Ricci, A. Garro, T. Juhász, I. Szigyártó, Z. Papp, G. Feresin, J. G. Torre, J. L. Cascales, L. Fülöp, **T. Beke-Somfai***, R. D. Enriz: New Short cationic antibacterial peptides. Synthesis, biological activity and mechanism of action, *BBA - Biomembranes*, **2021**, *1863*, 183665

IF: 3.4

- 25) G. Kohut, T. Juhász, M. Quemé-Peña, Sz. Bősze, **T. Beke-Somfai***: Controlling Peptide Function by Directed Assembly Formation: Mechanistic Insight using Multiscale Modelling on an Antimicrobial Peptide – Drug – Membrane system, *ACS Omega*, **2021**, *6*, 24, 15756–15769

IF: 3.512

- 26) 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

- 27) 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: 19.160

- 28) 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.*, **2021**, *4*, 1, 155-167

IF: 3.5

- 29) 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: 11.205

- 30) 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

- 31) 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

- 32) 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

- 33) A. Said-Ståhlsmiden, 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

- 34) 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

- 35) 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

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

IF: 5.880

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

IF: 16.971

- 38) F. Zsila, Sz. Bősze, **T. Beke-Somfai**: Interaction of antitubercular drug candidates with α 1-acid glycoprotein produced in pulmonary granulomas *Int. J. Biol. Macromol.* **2020**, *147*, 1318-1327

IF: 3.909

- 39) 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

- 40) F. Wang, X. Li, F. Zhang, X. Liu, P. Hu, **T. Beke-Somfai**, X. Lu: Revealing Interfacial Lipid Hydrolysis Catalyzed by Phospholipase A₁ at Molecular Level via Sum Frequency Generation Vibrational Spectroscopy and Fluorescence Microscopy, *Langmuir*, **2019**, *35*, 12831-12838

IF: 3.683

- 41) 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

- 42) 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 molecule suramin: a computational analysis *Phys. Chem. Chem. Phys.* **2019**, *21*, 10644-10659

IF: 3.906

- 43) 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

- 44) 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

- 45) 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
- 46) 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
- 47) 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
- 48) 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
- 49) 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
- 50) F. Zsila, T. Juhász, Sz. Bösze, 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
- 51) R. Kiss, M. Zhu, B. Jójárt, A. Czajlik, K. Solti, Balázs Fórizs, É. Nagy, F. Zsila, **T. Beke-Somfai**, G. Tóth: Structural Features of 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
- 52) F. Zsila, Sz. Bösze, 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
- 53) 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

- 54) 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
- 55) 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
- 56) 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
- 57) F. Zsila, **T. Beke-Somfai**: Dimeric Binding of Plant Alkaloid Ellipticine to Human Serum Proteins, *RSC Advances*, 2016, 6, 44096
IF: 3.289
- 58) 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
- 59) 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
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Book Chapters / Popular Scientific Articles

Paterson, A. J.; **Beke-Somfai, T.**; Kann, N., In *Science of Synthesis: Click Chemistry*, Rutjes, F. P. J. T., Ed.; Thieme: Stuttgart, (2021); p 289-335. DOI: 10.1055/sos-SD-235-00118

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*)

Selected Invited Oral Seminars at International Symposia

1. *June 2006, TAM Meeting-HPC Europa, Barcelona, Spain*, "A DFT Computational Investigation of the Catalytic Mechanism of Glutathione 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..."
8. *October, 2019, From Protein Complexes to Cell-Cell Communication, Esztergom Hungary*, "Extracellular vesicles as complex model systems for increased understanding on structure and function of membrane active proteins and peptides"
9. *September, 2018, 9th Chemistry towards Biology (CTB) Budapest, Hungary* "Complex peptide-membrane systems"
10. *October, 2021, 6th Polish-Korean Conference on Protein folding, Gdansk, Poland* "Design of Self-Assembling Foldamer Oligomers by Mimicking Natural Chirality Patterns"
11. *June, 2019. BIT's 12th Annual word protein and Peptide conference, Beijing, China* „Membrane Active Peptides"
12. *September, 2021, FilaVisu, Polymorphism of protein oligomers, Paris, France* "Spontaneous and induced assemblies of antimicrobial peptidic compounds"

Oral Presentation at International Symposia

May, 2007, Centenary Conference of the Hungarian Chemical Society, Sopron, Hungary
„From Amino acids to Nanotubes: Theoretical Investigation of beta-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)

May, 2019, Annual meeting ISEV 2019, Kioto, Japan, “Extracellular Vesicles for new Molecular Insight to Biomolecular Interactions”

May, 2020, Annual meeting ISEV 2020, (Online- Philadelphia, US) „Structural insight to interactions of extracellular vesicles and membrane active anticancer-antimicrobial peptides“

Selected Invited Presentations at Universities

Tokyo Institute of Technology, Tokyo, Japan, April 2019

Southeast University, Nanjing, China, August 2018

University of Twente, Twente, Netherlands, May 2016

Nanyang Technological University, Singapore, Singapore, February 2014

University of Southern Denmark, Odense, Denmark, February 2013

University of Oslo, Oslo, Norway, June 2013

Whitehead Institute, Massachusetts Institute of Technology, Boston, USA, August 2011

St. Jude’s Children Research Hospital, Memphis, USA, November 2010

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
Murray-Rust, P.; Thomas, J.; Echenique, P.; Hanwell, M.; Phadungsukanan, W.; Westerhoff, L.; **Beke-Somfai, T.**; Rzepa, H.; „Memex for computational chemistry”
Abstracts of Papers of the American Chemical Society 241, **2011**

June 2010, 35th FEBS Congress, Gothenburg, Sweden
Beke-Somfai, T.; Lincoln, P.; Nordén, B. „The reaction mechanism in ATPsynthase:

mechanical control by structural changes in the active sites" *Febs Journal*, 277, 274, **2010**

September 2004, 28th EPS, Prague, Czech Republic,

Beke, T.; Perczel, A. „Secondary structures of β -peptides: The unnatural behaviour of β -sheet" *Peptides Proceedings*, 700, **2005**

August 2002, 27th EPS, Sorrento, Italy,

Beke T. ; Perczel A. „Secondary Structures of beta-Peptides: The Unnatural Behaviour or beta-Sheets" *Journal of Peptide Science*, 10, 220, **2004**

Posters on International Symposia as Main Presenter: 30+