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| **C:\Users\user\Downloads\photo (1).jpg**Todor Dudev | Faculty of Chemistry and Pharmacy  Sofia University  1 James Bourchier Avenue  1164 Sofia, Bulgaria  tel. (+359 2) 8161 323  fax (+359 2) 9625 438  E-mail: t.dudev@chem.uni-sofia.bg |

**Areas of Expertise**

* Computational Chemistry/Biochemistry/Biophysics
* Metals in Biology and Medicine
* Molecular Modeling
* Coordination Chemistry
* Chemoinformatics
* Infrared and Raman Spectroscopy
* Teaching / Course Design

**Degrees**

**D.Sc. in Chemistry**

2015, *Sofia University, Bulgaria*

Thesis: “Factors Governing the Processes of Metal Binding and Selectivity in Metalloproteins and Ion Channels: In Silico Investigations”

**Ph.D. in Chemistry**1989, *Sofia University, Bulgaria*

Thesis: “Infrared Band Intensity Analysis: Algorithms and Applications”

**M.Sc. in Chemistry**

1984, *Sofia University, Bulgaria*

Graduated with Honors and received a Gold Medal for outstanding academic performance.

**Academic Positions**

**Professor in Chemistry** 2013 –

Faculty of Chemistry and Pharmacy

Sofia University, Bulgaria

**Senior Research Associate** 1997 – 2013

Institute of Biomedical Sciences

Academia Sinica, Taiwan

**Associate Professor** 1997 – 2000

Department of Chemistry

Sofia University, Bulgaria

**Assistant Professor** 1989 – 1997

Department of Chemistry

Sofia University, Bulgaria

**Sabbaticals and International Grants**

**Visiting Professor** Spring 2014, 2015, 2018

Universidad de Alcala de Henares

Alcala de Henares, Spain

**Visiting Professor** Autumn 2012

Laboratoire de Pharmacochimie Moleculaire et Cellulaire

University Paris – Descartes

Paris, France

**Visiting Scientist** Summer 1999, Autumn 1993

Instituto de Estructura de la Materia

Consejo Superior de Investigaciones Cientificas

Madrid, Spain

**Visiting Scientist** Summer 1996

College of Arts & Sciences

University of Missouri-Kansas City

Kansas City, MO, USA

**Visiting Scientist** Winter 1994, Spring 1996

Department of Analytical Chemistry

Dresden University of Technology,

Dresden, Germany

**Visiting Scientist** Summer 1993

Department of Chemistry & Applied Chemistry

University of Salford,

Manchester, UK

**Postdoctoral Researcher** 10/1989 – 9/1990

Research Laboratory of Resources Utilization,

Tokyo Institute of Technology

Tokyo, Japan

**Invited Talks**

* Second PRESTO Meeting on P2X receptors – a common route in different diseases: preclinical and clinical aspects, Pisa, Italy, 2023.
* First PRESTO COST Action CA21130 Meeting, P2X receptors as therapeutic targets, Ferrara, Italy, 2023.
* 27th Lecture Session on Modern Directions of Natural Sciences, Sofia University, Bulgaria, 2021.
* Workshop “Advanced Materials”, St. St. Constantine and Helena, Bulgaria, 2019.
* PRACE Winter School 2018 – Computational Chemistry, Biochemistry and Medicinal Chemistry – Methods and Tools, Sofia, Bulgaria, 2018.
* The 13th Workshop with International Participation: Biological Activity of Metals, Synthetic Compounds and Natural Products, Sofia, Bulgaria, 2018.
* Workshop “Advanced Materials”, Duni, Bulgaria, 2018.
* Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Czech Republic, 2018.
* Departament de Nutricio, Ciencies de l’Alimentacio i Gastronomia, Universitat de Barcelona, Spain, 2017.
* Conference on Modeling Interactions in Biomolecules VIII, Pilsen, Czech Republic, 2017.
* Workshop “Advanced Materials”, Pomorie, Bulgaria, 2017.
* 3rd Symposium on Weak Molecular Interactions, Opole, Poland, 2017.
* Department of Chemistry, Jagiellonian University, Krakow, Poland, 2017.
* The Third International Conference on Computational Science and Engineering, Ho Chi Minh City, Vietnam, 2016.
* Department of Organic Chemistry, The Hebrew University of Jerusalem, Israel, 2016.
* Workshop “Advanced Functional Materials”, Pravets, Bulgaria, 2016.
* Tenth Workshop on Biological Activity of Metals, Synthetic Compounds and Natural Products, Sofia, Bulgaria, 2015.
* Unidad Docente de Quimica Fisica, Universidad de Alcala de Henares, Alcala de Henares, Spain, 2014, 2015, 2018.
* Scientific Session of the Faculty of Chemistry and Pharmacy, Sofia University, Sofia, Bulgaria, 2015.
* Workshop “Applied Research on Functional Materials”, Velingrad, Bulgaria, 2014.
* Conference on Modeling Interactions in Biomolecules VI, Marianske Lazne, Czech Republic, 2013.
* Workshop “Fundamental and Applied, Approved and New Research Methods with Biomedical Application”, Pravets, Bulgaria, 2013.
* 17th Biophysics Conference, Taipei, Taiwan, 2012.
* Laboratoire de Pharmacochimie Moleculaire et Cellulaire, University Paris – Descartes, France, 2012.
* Structural Bioinformatics Division, Institute Pasteur, Paris, France, 2012
* Laboratoire de Biochimie Theorique, Institute de Biologie Physico-Chimique, Paris, France, 2012.
* Conference on Modeling Interactions in Biomolecules V, Kutna Hora, Czech Republic, 2011.
* Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan, 2011.
* 2nd Annual International Conference on Computational and Systems Biology, Hangzhou, China, 2010.
* 1st Workshop on Multiscale Simulations of Biological Molecules, Taipei, Taiwan, 2010.
* Conference on Modeling Interactions in Biomolecules IV, Hruba Skala, Czech Republic, 2009.
* Conference on Viral Membrane Proteins, Heidelberg, Germany, 2008.
* 12th International Conference on Theoretical Aspects of Catalysis, Varna, Bulgaria, 2008.
* 3rd Asian Pacific Conference on Theoretical and Computational Chemistry, Beijing, China, 2007.
* 3rd Humboldt Conference on Computational Chemistry, Varna, Bulgaria, 2006.
* Modeling Interactions in Biomolecules II, Prague, Czech Republic, 2005.
* Modeling Interactions in Biomolecules, Nove Hrady, Czech Republic, 2003.
* XXIII European Congress on Molecular Spectroscopy, Balatonfured, Hungary, 1996

**Manuscript Reviewer**

* Journal of the American Chemical Society
* Journal of Physical Chemistry
* Zeitschrift fur Anorganische und Allgemeine Chemie
* Journal of Computer-Aided Molecular Design
* Journal of the Chinese Chemical Society
* Journal of Molecular Modeling
* BioMetals
* Journal of Molecular Graphics and Modeling
* Spectrochimica Acta
* Journal of Molecular Structure
* Metallomics
* Physical Chemistry Chemical Physics
* Journal of Organic Chemistry
* Inorganic Chemistry
* Chemical Science
* Molecules

**Member of the Editorial Board of the journal “Computational Chemistry”**

**Member of the Editorial Board of the journal “World Journal of Methodology”**

**Member of the Editorial Board of the journal “Frontiers in Pharmacology”**

**Member of the Editorial Board of the journal "EUREKA: Life Sciences”**

**Grant-Proposal Evaluator for the European Research Council (Consolidated Grants) 2016-2022**

**Participant in COST action “P2X receptors as a therapeutic opportunity” 2022-**

**Awards:**

**“Pythagoras” award for exceptional achievements in the field of natural and engineering sciences (Bulgaria, 2017)**

**“Pythagoras” grand prize for overall scientific contribution (Bulgaria, 2023)**

**Publications**

One book, 3 book chapters and 142 research papers. *Please refer to the attached list for a complete record of all publications.*

Total number of citations (without self-citations): 4000

H-index: 32 (WoS) and 36 (Google Scholar)

**Teaching Experience**

**University Courses Taught**

2013 - *Ab initio MO Calculations* – Sofia University, Bulgaria

2013 - *Computational Methods in Spectroscopy* – Sofia University, Bulgaria

2013 - *Instrumental Methods in Chemistry* – Sofia University, Bulgaria

2013 - *Pharmaceutical Analysis –* Sofia University, Bulgaria

2015 – *Biochemistry* – Sofia University, Bulgaria

2006 *Protein Biochemistry* – National Yang Ming University, Taiwan

2006 *Medicinal Chemistry* – National Yang Ming University, Taiwan

1991 – 1997 *Applied Spectroscopy* – Sofia University, Bulgaria

1991 – 1997 *Spectroscopy of Biologically Active Molecules* – Sofia University,

Bulgaria

1987 – 1997 *Quantum Chemistry and Spectroscopy* – Sofia University, Bulgaria

**Distance Learning**

Pioneered distance learning in Bulgaria together with a team of other Sofia University researches. Worked as a member of the National Contact Point, National Centre for Distance Education, Subcontractor for Bulgaria of the PHARE Multi-Country Program for Distance Education, 1995-1997. Developed distance learning programs, materials and methodologies that were among the first in Eastern Europe.

Todor Dudev

List of Publications

**Book**

B. Galabov and T. Dudev, “Vibrational Intensities”, Elsevier, Amsterdam, 1996 (342 pages).

**Book Chapters**

C. Lim and T. Dudev, "Potassium Versus Sodium Selectivity in Monovalent Ion Channel Selectivity Filters” in *The Alkali Metal Ions: Their Role for Life*, Vol. 16 of Metal Ions in Life Sciences (Eds. A. Sigel, H. Sigel, R.K.O. Sigel), Springer International, Cham, Switzerland, 2016, pp. 325-347.

T. Dudev and C. Lim, “Calcium Ion Selectivity in Biological Systems”, in *Encyclopedia of Metalloproteins* (V.N. Uversky, R.H. Kretsinger, E.A. Permyakov, Eds.), Springer Science, New York, 2013, pp. 478-484.

B. Galabov, T. Dudev and J.R. Durig, “Molecular Conformation from Vibrational Intensity Analysis”, in *Progress in Molecular Spectroscopy* (R. Salzer, H. Kriegsmann, G. Werner, Eds.), Teubner, Leipzig, 1988, p. 113.

**Papers**

* *Reviews*

1. T. Dudev, “How theoretical evaluations can generate guidelines for designing/engineering metalloproteins with desired metal affinity and selectivity”, *Molecules* **28** (2023) 249.
2. T. Dudev, C. Grauffel and C. Lim, “Calcium in Signaling: Its Specificity and Vulnerabilities toward

Biogenic and Abiogenic Metal Ions”, *J. Phys. Chem. B* **125** (2021) 10419-10431.

1. N. Kircheva and T. Dudev, „Competition between abiogenic and biogenic metal cations in biological systems: Mechanisms of gallium‘s anticancer and antibacterial effect“, *J. Inorg. Biochem.* **214** (2021) 111309.
2. T. Dudev, K. Mazmanian, W.-H. Weng, C. Grauffel and C. Lim, “Free and bound lithium in brain signaling“, *Acc. Chem. Res*. **52** (2019) 2960-2970.
3. N. Kircheva and T. Dudev, “Mechanism of therapeutic action of abiogenic Li+ and Ga3+ ions: Insights from theoretical studies”, *Bulg. Chem. Commun*. **50** (2018) 55-62.
4. T. Dudev and C. Lim, “Competition among Metal Ions for Protein Binding Sites: Determinants of Metal Ion Selectivity in Proteins”, *Chem. Rev*. **114** (2014) 538-556.
5. D. Meffre, J. Grenier, S. Bernard, F. Courtin, T. Dudev, G.G. Shackleford, M. Jafarian-Tehrani and C. Massaad, “Wnt and Lithium: a Common Destiny in the Therapy of Nervous System Pathologies?”, *Cell. Mol. Life Sci.* **71** (2014) 1123-1148.
6. T. Dudev and C. Lim, “Ion Selectivity Strategies of Sodium Channel Selectivity Filters”, *Acc. Chem. Res.* **47** (2014) 3580-3587.
7. T. Dudev and C. Lim, “Metal Binding and Selectivity in Metalloproteins: Insights from Computational Studies”, *Annual Review of Biophysics* **37** (2008) 97-116.
8. T. Dudev and C. Lim, “Effect of Carboxylate-Binding Mode on Metal Binding/Selectivity and Function in Proteins”, *Acc. Chem. Res.* **40** (2007) 85-93.
9. T. Dudev and C. Lim, “Principles Governing Mg, Ca and Zn Selectivity in Proteins”, *Chem. Rev.* **103** (2003) 773 – 787.
10. T. Dudev and C. Lim, “Metal Binding and Selectivity in Zinc Proteins”, *J. Chin. Chem. Soc.* **50** (2003) 1093-1102.

* *Journal Articles*

1. T. Sarafska , S. Ivanova , T. Dudev , V. Petrov and T. Spassov, “Beta-cyclodextrin – Citric acid complexation by ball milling and annealing”, *J. Mol. Struct*. **1295** (2024) 136701.
2. N. Kircheva, V. Petkova, S. Dobrev, V. Nikolova, S. Angelova and T. Dudev, “N-Methyl- and N-Phenylpiperazine Functionalized Styryl Dyes inside Cucurbiturils: Theoretical Assessment of the Factors Governing the Host-Guest Recognition”, *Molecules* **28** (2023) 8130.
3. S. Angelova, N. Kircheva, V. Nikolava, S. Dobrev and T. Dudev, “Electrostatic interactions - key determinants of the metal selectivity in La3+ and Ca2+ binding proteins”, *Phys. Chem. Chem. Phys*. **25** (2023) 18149-18157.
4. K. Mazmanian, C. Grauffel, T. Dudev and C. Lim, “Protein Ca2+ -Sites Prone to Sr2+ Substitution: Implications for Strontium Therapy” *J. Phys. Chem. B* **127** (2023) 5588-5600.
5. N. Kircheva, S. Angelova, S. Dobrev, V. Petkova, V. Nikolova and T. Dudev, “Cu+/Ag+ Competition in Type I Copper Proteins (T1Cu)”, *Biomolecules* **13** (2023) 681.
6. V. Petkova, V. Nikolova, N. Kircheva, S. Dobrev, S. Angelova and T. Dudev, “Theoretical study of β-cyclodextrin inclusion complexes with vitamin K”, *Innovations* **11** (2023) 37-40.
7. V. Nikolova, N. Kircheva, S. Dobrev, S. Angelova and T. Dudev, “Lanthanides as Calcium Mimetic Species in Calcium-Signaling/Buffering Proteins: The Effect of Lanthanide Type on the Ca2+/Ln3+ Competition”, *Int. J. Mol. Sci*. **24** (2023) 6297.
8. N. Kircheva, S. Dobrev, V. Petkova, V. Nikolova, S. Angelova and T. Dudev, “Complexation of metal cations (mono-, di- and trivalent) to cucurbiturils: Insights from a DFT/SMD study”, *Int. Sci. J. Science. Business. Society* **8** (2023) 3-6.
9. N. Kircheva, S. Dobrev, L. Dasheva, V. Nikolova, S. Angelova and T. Dudev, “Metal-assisted complexation of fluorogenic dyes by cucurbit[7]uril and cucurbit[8]uril: a DFT/SMD evaluation of the key factors governing the host–guest recognition”, *Molecules* **28** (2023) 1540.
10. V. Nikolova, S. Dobrev, N. Kircheva, V. Yordanovа, T. Dudev and S. Angelova, “Host-guest complexation of cucurbit[7]uril and cucurbit[8]uril with the antimuscarinic drugs tropicamide and atropine”, *J. Mol. Graph. Modell.*, **119** (2023) 108380.
11. S. Dobrev, N. Kircheva, V. Nikolova, S. Angelova and T. Dudev, “Competition between Ag+ and Ni2+ in nickel enzymes: Implications for the Ag+ antibacterial activity”, *Comp. Biol. Chem*. **101** (2022) 107785.
12. N. Kircheva, V. Nikolova, S. Dobrev, S. Angelova and T. Dudev, “β-Cyclodextrin-modulated interaction of Gd3+ with levofloxacin: a molecular modeling study”, *Trends Phys. Chem*. **22** (2022) 39-49.
13. N. Kircheva, N. Toshev and T. Dudev, ”Holo-chromodulin: Competition between the native Cr3+ and other biogenic cations (Fe3+, Fe2+, Mg2+ and Zn2+) for the binding sites”, *Metallomics* **14** (2022) mfac082.
14. N. Kircheva, S. Dobrev, V. Nikolova, S. Angelova and T. Dudev, “Theoretical Insight into the Phosphate-Targeted Silver’s Antibacterial Action: Differentiation between Gram (+) and Gram (-) Bacteria“, *Inorg. Chem*. **61** (2022) 10089-10100.
15. N. Kircheva, S. Dobrev, V. Nikolova, S. Angelova and T. Dudev, “Abiogenic Metals in Medicine. Insights from Theoretical Studies of the Mechanisms of Action of Silver (I), Strontium (II), and Gallium (III)”, *Int. Sci. J. Science. Business. Society* **7** (2022) 3-6.
16. I.Z. Koleva, S. Dobrev, N. Kircheva, L. Dasheva, V. Nikolova, S. Angelova and T. Dudev, „Complexation of trivalent metal cations (Al3+, Ga3+, In3+, La3+, Lu3+) to cucurbiturils: a DFT/SMD evaluation of the key factors governing the host–guest recognition“, *Phys. Chem. Chem. Phys*., **24** (2022) 6274.
17. T. Dudev, D. Cheshmedzhieva, P. Dorkov and I. Pantcheva, “A DFT/PCM Study on the Affinity of Salinomycin to Bind Monovalent Metal Cations”, *Molecules* **27** (2022) 532.
18. D. Cheshmedzhieva, S. Ilieva, E.A. Permyakov, S.E. Permyakov and T. Dudev, „Ca2+/Sr2+ Selectivity in Calcium-Sensing Receptor (CaSR): Implications for Strontium’s Anti-Osteoporosis Effect“, *Biomolecules* **11** (2021) 1576.
19. A.A. Vologzhannikova, M.P. Shevelyova, A.S. Kazakov, A.S. Sokolov, N.I. Borisova, E. A. Permyakov, N. Kircheva, V. Nikolova, T. Dudev and S.E. Permyakov, “Strontium Binding to   
    α-Parvalbumin, a Canonical Calcium-Binding Protein of the “EF-Hand” Family”, *Biomolecules* **11** (2021) 1158.
20. C. Grauffel, W.-H. Weng, T. Dudev, and C. Lim, "The Trinuclear Calcium Site in the C2 domain of PKCα/γ is Prone to Lithium Attack", *ACS Omega* **6** (2021) 20657-20666.
21. N. Toshev, D. Cheshmedzhieva and T. Dudev, "Factors governing the affinity and selectivity of histone deacetylase inhibitors for the HDAC8 enzyme active site: Implications for anticancer therapy", *J. Phys. Org. Chem.* **34** (2021) e4268.
22. D. Damyanov, V. Nikolova, S. Angelova and T. Dudev, “Halide anion solvation and recognition by bambusurils: a DFT study”, *J. Mol. Liq.* **335** (2021) 116160.
23. C. Grauffel, T. Dudev and C. Lim, “Metal Affinity/Selectivity of Monophosphate-Containing Signaling/Lipid Molecules”, *J. Chem. Theor. Comput*. **17** (2021) 2444-2456.
24. V. Nikolova, A. Velinova, S. Dobrev, N. Kircheva, S. Angelova and T. Dudev, “Host−Guest Complexation of Cucurbit[7]Uril and Cucurbit[8]Uril with the Antineoplastic and Multiple Sclerosis Agent Mitoxantrone (Novantrone)”, *J. Phys. Chem. A* **125** (2021) 536-542.
25. N. Kircheva, S. Dobrev, V. Nikolova, S. Angelova, and T. Dudev, “Zinc and Its Critical Role in Retinitis pigmentosa: Insights from DFT/SMD Calculations”, *Inorg. Chem*. **59** (2020) 17347-17355.
26. N. Kircheva, S. Dobrev, L. Dasheva, I. Koleva, V. Nikolova, S. Angelova and T. Dudev, “Complexation of biologically essential (mono- and divalent) metal cations to cucurbiturils: A DFT/SMD evaluation of the key factors governing the host-guest recognition”, *RSC Advances* **10** (2020) 28139-28147.

1. S. Yordanova-Tomova, D. Cheshmedzhieva, S. Stoyanov, T. Dudev and I. Grabchev, „Synthesis, Photophysical Characterization, and Sensor Activity of new 1,8-Naphtalimide Derivatives“, *Sensors* **20** (2020) 3892.
2. N. Kircheva and T. Dudev, “Gallium as an Antibacterial Agent: A DFT/SMD Study of the Ga3+/Fe3+ Competition for Binding Bacterial Siderophores”, *Inorg. Chem*. **59** (2020) 6242-6254.
3. T. Dudev, D. Cheshmedzhieva, R. Dimitrova, P. Dorkov and I. Pantcheva, “Factors governing the competition between group IA and IB cations for monensin A: a DFT/PCM study”, *RSC Advances* **10** (2020) 5734-5741.
4. T. Dudev, L.M. Frutos and O. Castano, “How mechanical forces can modulate the metal affinity and selectivity of metal binding sites in proteins”, *Metallomics* **12** (2020) 363-370.
5. S. Pereva, V. Nikolova, T. Sarafska, S. Angelova, T. Spassov, T. Dudev, “Inclusion complexes of ibuprofen and β-cyclodextrin: Supramolecular structure and stability”, *J. Mol. Struct*. **1205** (2020) 127575.
6. C. Grauffel, T. Dudev and C. Lim, „Why Cellular Di/Triphosphates Preferably Bind Mg2+ and Not Ca2+, *J. Chem. Theor. Comput*. **15** (2019) 6992-7003.
7. S. Ilieva, D. Cheshmedzhieva and T. Dudev, “Electric field influence on the helical structure of peptides: insights from DFT/PCM computations”, *Phys. Chem. Chem. Phys*. **21** (2019) 16198-16206.
8. S. Pereva, V. Nikolova, S. Angelova, T. Spassov and T. Dudev, “Water inside β-cyclodextrin cavity: amount, stability and mechanism of binding”, *Beilstein J. Org. Chem*. **15** (2019) 1592-1600.
9. N. Kircheva and T. Dudev, “Novel insights into gallium’s mechanism of therapeutic action: a DFT/PCM study of the interaction between Ga3+ and ribonucleotide reductase substrates*”, J. Phys. Chem. B* **123** (2019) 5444-5451.
10. V.K. Nikolova, C.V. Kirkova, S.E. Angelova and T.M. Dudev, “Host-guest interactions between p-sulfonatocalix[4]arene and p-sulfonatothiacalix[4]arene and group IA, IIA and f-block metal cations: a DFT/SMD study”, *Beilstein J. Org. Chem.* **15** (2019) 1321-1330.
11. T. Dudev, C. Grauffel and C. Lim, “How Pb2+ Binds and Modulates Properties of Ca2+-Signaling Proteins”, *Inorg. Chem.* **57** (2018) 14798-14809.
12. T. Dudev, S. Ilieva and L. Doudeva, ”How an electric field can modulate the metal ion selectivity of protein binding sites: insights from DFT/PCM calculations”, *Phys. Chem. Chem. Phys*. **20** (2018) 24633-24640.
13. K. Mazmanian, T. Dudev and C. Lim, “How first shell – second shell interactions and metal substitution modulate protein function”, *Inorg. Chem*. **57** (2018) 14052-14061.
14. S. Angelova, V. Nikolova and T. Dudev, “Divalent metal ions binding to lactose: a DFT computational study”, *Bulg. Chem. Commun*. **50** (2018) 130-134.
15. D. Cheshmedzhieva, N. Toshev, M. Gerova, O. Petrov and T. Dudev, “Sulfur and selenium derivatives of suberoyl anilide hydroxamic acid (SAHA) as a plausible HDAC inhibitors: a DFT study of their tautomerism and metal affinity/selectivity”, *Bulg. Chem. Commun*. **50** (2018) 228-236.
16. T. Dudev, C. Grauffel, S.-T. D. Hsu and C. Lim, “How native and non-native cations bind and modulate the properties of GTP/ATP”, *J. Chem. Theor. Comput*. **14** (2018) 3311-3320.
17. T. Dudev, K. Mazmanian and C. Lim, “Competition between Li+ and Na+ in sodium transporters and receptors: Which Na+-binding sites are “therapeutic” Li+ targets?”, *Chem. Sci.* **9** (2018) 4093-4103.
18. D. Cheshmedzhieva, N. Toshev, M. Gerova, O. Petrov and T. Dudev, “Hydroxamic acid derivatives as histone deacetylase inhibitors: a DFT study of their tautomerism and metal affinities/selectivities”, *J. Mol. Modeling* **24** (2018) 114.
19. T. Dudev, D. Cheshmedzhieva and L. Doudeva, “Competition between abiogenic Al3+ and native Mg2+, Fe2+ and Zn2+ ions in protein binding sites: Implications for aluminium toxicity”, *J. Mol. Modeling* **24** (2018) 55.
20. S. Angelova, V. Nikolova, S. Pereva, T. Spassov and T. Dudev, “α-Cyclodextrin: How Effectively Can Its Hydrophobic Cavity Be Hydrated?”, *J. Phys. Chem. B* **121** (2017) 9260-9267.
21. V. Nikolova, S. Angelova and T. Dudev, ”IIA/IIB group metal cations hosted by β-cyclodextrin: a DFT study”, *Bulg. Chem. Commun*. **49** (2017) 189-194.
22. S.E. Angelova, V.K. Nikolova and T.M. Dudev, “Determinants of the host-guest interactions between α-, β- and γ-cyclodextrins and group IA, IIA and IIIA metal cations: a DFT/PCM study”, *Phys. Chem. Chem. Phys.* **19** (2017) 15129-15136.
23. S. Angelova, V. Nikolova, N. Molla and T. Dudev, “Factors Governing the Host−Guest Interactions between IIA/IIB Group Metal Cations and α‑Cyclodextrin: A DFT/CDM Study”, *Inorg. Chem*. **56** (2017) 1981-1987.
24. T. Dudev, C. Grauffel and C. Lim, “How Native and Alien Metal Cations Bind ATP: Implications for Lithium as a Therapeutic Agent”, *Sci. Rep.* **7** (2017) 42377.
25. T. Dudev and L. Doudeva, “How the extra methylene group affects the ligation properties of Glu vs. Asp and Gln vs. Asn amino acids: a DFT/PCM study”, *J. Mol. Modeling* **23** (2017) 45.
26. T. Dudev and V. Nikolova, “Determinants of Fe2+ over M2+ (M = Mg, Mn, Zn) Selectivity in Non-Heme Iron Proteins”, *Inorg. Chem.* **55** (2016) 12644–12650.
27. K. Mazmanian, K. Sargsyan, C. Grauffel, T. Dudev, and C. Lim, “Preferred Hydrogen-Bonding Partners of Cysteine: Implications for Regulating Cys Functions”, *J. Phys. Chem. B* **120** (2016) 10288–10296.
28. T. Dudev, C. Grauffel and C. Lim, “Influence of the Selectivity Filter Properties on Proton Selectivity in the Influenza A M2 Channel”, *J. Am. Chem. Soc*. **138** (2016) 13038-13047.
29. T. Dudev, K. Mazmanian, and C. Lim, “Factors controlling the selectivity for Na+ over Mg2+ in sodium transporters and enzymes”, *Phys. Chem. Chem. Phys.* **18** (2016) 16986-16997.
30. V. Nikolova, S. Angelova, N. Markova, and T. Dudev, “Gallium as a Therapeutic Agent: A Thermodynamic Evaluation of the Competition between Ga3+ and Fe3+ Ions in Metalloproteins”, *J. Phys. Chem. B* **120** (2016) 2241-2248.
31. S. Pereva, T. Himitliiska, T. Spassov, S.D. Stoyanov, L.N. Arnaudov and T. Dudev, “Cyclodextrin-Based Solid-Gas Clathrates”, *J. Agric. Food Chem*. **63** (2015) 6603-6613.
32. T. Dudev, B. Musset, D. Morgan, V.V. Cherny, S.M.E. Smith, K. Mazmanian, T.E. DeCoursey and C. Lim, “Selectivity Mechanism of the Voltage-gated Proton Channel, HV1”, *Sci. Rep.* **5** (2015) 10320.
33. T. Dudev and C. Lim, “Ion Selectivity in the Selectivity Filters of Acid-Sensing Ion Channels”, *Sci. Rep.* **5** (2015) 7864.
34. T. Dudev, M. Devereux, M. Meuwly, C. Lim, J.-P. Piquemal and N. Gresh, “Quantum-Chemistry Based Calibration of the Alkali Metal Cation Series (Li+-Cs+) for Large-Scale Polarizable Molecular Mechanics/Dynamics Simulations”, *J. Comp. Chem.* **36** (2015) 285-302.
35. C.S. Babu, Y.-M. Lee, T. Dudev and C. Lim, “Modeling Zn2+ Release from Metallothionein”, *J. Phys. Chem. A* **118** (2014) 9244-9252.
36. T. Dudev, “Modeling Metal Binding Sites in Proteins by Quantum Chemical Calculations”, *Comp. Chem*. **2** (2014) 19-21.
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