

AMR-TB Publications

1. Ugo Bastolla, Mikhail Rotkevich, Miguel Arenas, Manuel Arrayas, Marine Dogonadze, Anastasia Lavrova, Molina-Jorge Sejas, Michael Tadesse, Xulvi-Ramon Brunet, Jonathan Cox, Dmitry Nerukh, Gonzalez-Natalia Benitez, and Michael Stich, **Fitness Effect of the Isoniazid Resistance Mutation S315T of the Catalase-Peroxidase Enzyme KatG of Mycobacterium tuberculosis**, *Genome Biology and Evolution*, **17** (7), evaf120 (2025),
2. M. Bakumenko, V. Bardik, V. Farafonov, and D. Nerukh, **The Multiscale Hybrid Method with a Localized Constraint. II. Hybrid Equations of Motion Based on Variational Principles**, *Ukrainian Journal of Physics*, **69** (4), 269 (2024).
3. Anna Laguta, Natalya Vodolazkaya, and Dmitry Nerukh, **The Spectrophotometric Determination of the Patchy Surface Potential of Viruses Using pH-Sensitive Molecular Probes**, *J. Chem. Educ.*, **101** (3), 1190-1197 (2024),
4. Sergey A. Karabasov, Mihail A. Zaitsev, and Dmitry A. Nerukh, **The nut-and-bolt motion of a bacteriophage sliding along a bacterial flagellum: a complete hydrodynamics model**, *Scientific Reports*, **13** (1), 9077 (2023),
Open access full text at <https://rdcu.be/ddLVg>,
5. Natalya Vodolazkaya, Anna Laguta, Vladimir Farafonov, Marina Nikolskaya, Zita Balklava, Reza Khayat, Michael Stich, Nikolay Mchedlov-Petrosyan, and Dmitry Nerukh, **Influence of various colloidal surfactants on the stability of MS2 bacteriophage suspension. The charge distribution on the PCV2 virus surface**, *Journal of Molecular Liquids*, **387**, 122644 (2023),
6. Vladimir S. Farafonov, Michael Stich, and Dmitry A. Nerukh, **Complete Virion Simulated: All-Atom Model of an MS2 Bacteriophage with Native Genome**, *Journal of Chemical Theory and Computation*, **19** (21), 7924-7933 (2023),
7. M. Bakumenko, V. Bardik, and D. Nerukh, **The Multiscale Hybrid Method with a Localized Constraint. I. A Modified Control Volume Function for the Hybridized Mass and Momentum Equations**, *Ukrainian Journal of Physics*, **68** (8), 517 (2023),
8. Vladimir S. Farafonov, Alexander V. Lebed, Dmitry A. Nerukh, and Nikolay O. Mchedlov-Petrosyan, **Estimation of Nanoparticle's Surface Electrostatic Potential in Solution Using Acid-Base Molecular Probes I: In Silico Implementation for Surfactant Micelles**, *The Journal of Physical Chemistry B*, **126** (4), 1022-1030 (2023),
9. Vladimir S. Farafonov, Alexander V. Lebed, Dmitry A. Nerukh, and Nikolay O. Mchedlov-Petrosyan, **Estimation of Nanoparticle's Surface Electrostatic Potential in Solution Using Acid-Base Molecular Probes II: Insight from Atomistic Simulations of Micelles**, *The Journal of Physical Chemistry B*, **126** (4), 1031-1038 (2023),
10. Natalya Vodolazkaya, Marina Nikolskaya, Anna Laguta, Vladimir Farafonov, Zita Balklava, Michael Stich, Nikolay Mchedlov-Petrosyan, and Dmitry Nerukh, **Estimation of Nanoparticle's Surface Electrostatic Potential in Solution Using Acid-Base Molecular Probes. III. Experimental Hydrophobicity/Hydrophilicity and Charge Distribution of MS2 Virus Surface**, *The Journal of Physical Chemistry B*, **126** (41), 8166-8176 (2022),
11. Vladimir S. Farafonov, Michael Stich, and Dmitry Nerukh, **Reconstruction and validation of entire virus model with complete genome from mixed resolution cryo-EM density**, *Faraday Discuss.*, **240**, 152-167 (2022),

12. Ekaterina Maximova, Eugene B. Postnikov, Anastasia I. Lavrova, Vladimir Farafonov, and Dmitry Nerukh,
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13. Elvira Tarasova, Noriaki Okimoto, Shanshan Feng, Dmitry Nerukh, Reza Khayat, and Makoto Taiji,
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14. N. Atamas, V. Bardik, O. Grishina, S. Komisarenko, E. Lugovskoi, S. Lavoryk, N. Malomuzh, Y. Makogonenko, and D. Nerukh,
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15. Ye. M. Makogonenko, V. O. Chernyshenko, V. Yu. Bardyk, A. V. Udovenko, and S. V. Komisarenko,
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<https://doi.org/10.15407/ubj97.01.075>.
16. Konstantin N. Semenov, Ali Mlhem, Alexander V. Akentiev, Dmitry A. Nerukh, Natalia V. Petukhova, Ilnaz T. Rakipov, Kirill V. Timoshchuk, Gleb O. Iurev, Andrey V. Petrov, Igor V. Murin, Nikolay A. Charykov, Olga S. Vezo, Anastasia V. Penkova, Dilafruz K. Kholmurodova, Jasur A. Rizaev, Aziz S. Kubaev, and Vladimir V. Sharoyko,
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