Сведения о научном руководителе
по диссертации *Метелешко Юлии Игоревны*
«Молекулярное моделирование мутантных форм флуоресцентных белков на основе LOV доменов с измененными спектральными свойствами»

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Список основных научных публикаций по специальности 1.4.4 – физическая химия за последние 5 лет:

1. *Krivitskaya A. V., Khrenova M. G.* Evolution of ceftriaxone resistance of penicillin-binding proteins 2 revealed by molecular modeling // *International Journal of Molecular Sciences*. — 2023. — Vol. 24, no. 1. — P. 176
2. Extracellular fe(iii) reductase structure reveals a modular organization enabling s-layer insertion and electron transfer to insoluble substrates / T. V. Tikhonova, E. M. Osipov, N. I. Dergousova et al. // *Structure*. — 2023. — Vol. 31, no. 2. — P. 174–184.
3. Complex of hiv-1 integrase with cellular ku protein: Interaction interface and search for inhibitors / E. Ilgova, S. Galkin, M. Khrenova et al. // *International Journal of Molecular Sciences*. — 2022. — Vol. 23. — P. 2908.
4. Drug repurposing of the unithiol: Inhibition of metallo-beta-lactamases for the treatment of carbapenem-resistant gram-negative bacterial infections / V. G. Grigorenko, M. G. Khrenova, I. P. Andreeva et al. // *International Journal of Molecular Sciences*. — 2022. — Vol. 23, no. 3. — P. 1834.
5. Nanopore sequencing for de novo bacterial genome assembly and search for single-nucleotide polymorphism / M. G. Khrenova, T. V. Panova, V. A. Rodin et al. // *International Journal of Molecular Sciences*. — 2022. — Vol. 23, no. 15. — P. 8569.
6. *Khrenova M. G., Mulashkin F. D., Nemukhin A. V.* Modeling spectral tuning in red fluorescent proteins using the dipole moment variation upon excitation // *Journal of Chemical Information and Modeling*. — 2021. — Vol. 61, no. 10. — P. 5125–5132
7. *Khrenova M. G., Grigorenko B. L., Nemukhin A. V.* Molecular modeling reveals the mechanism of ran-rangap-catalyzed guanosine triphosphate hydrolysis without an arginine finger // *ACS catalysis*. — 2021. — Vol. 11, no. 15. — P. 8985–8998.
8. The o to s substitution in urea brings inhibition activity against thiocyanate dehydrogenase / M. G. Khrenova, A. Y. Soloveva, T. V. Tikhonova, V. O. Popov // *Mendeleev Communications*. — 2021. — Vol. 31. — P. 373–375.
9. The role of cysteine residues in the allosteric modulation of the chromophore phototransformations of biphotochromic fluorescent protein saasoti / A. V. Gavshina, N. K. Marynich, M. G. Khrenova et al. // *Scientific reports*. — 2021. — Vol. 11. — P. 24314
10. Dipole moment variation clears up electronic excitations in the π-stacked complexes of fluorescent protein chromophores / M. G. Khrenova, F. D. Mulashkin, E. S. Bulavko et al. // *Journal of Chemical Information and Modeling*. — 2020. — Vol. 60, no. 12. — P. 6288.

11. *Khrenova M. G., Tsirelson V. G., Nemukhin A. V.* Dynamical properties of enzyme–substrate complexes disclose substrate specificity of the sars-cov-2 main protease as characterized by the electron density descriptors // *Physical Chemistry Chemical Physics*. — 2020. — Vol. 22 — P. 19069.
12. *Khrenova M. G., Kulakova A. M., Nemukhin A. V.* Proof of concept for poor inhibitor binding and efficient formation of covalent adducts of krasg12c and ars compounds // *Organic and Biomolecular Chemistry*. — 2020. — Vol. 18 — P. 3069.
13. *Kots E. D., Khrenova M. G., Nemukhin A. V.* Allosteric control of n-acetyl-aspartate hydrolysis by the y231c and f295s mutants of human aspartoacylase // *Journal of Chemical Information and Modeling*. — 2019. — Vol. 59, no. 5. — P. 2299–2308.
14. Computational challenges in modeling of representative bioimaging proteins: Gfp-like proteins, flavoproteins, and phytochromes / A. V. Nemukhin, B. L. Grigorenko, M. G. Khrenova, A. I. Krylov // *Journal of Physical Chemistry B*. — 2019. — Vol. 123, no. 29. — P. 6133–6149.
15. *Meteleshko Y. I., Nemukhin A., Khrenova M.* Novel flavin-based fluorescent proteins with red-shifted emission bands: a computational study // *Photochemical and Photobiological Sciences*. — 2019. — Vol. 18. — P. 177–189.

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