

**Избранные публикации официального оппонента
доктора физико-математических наук, профессора РАН
ХРЕНОВОЙ Марии Григорьевны
по тематике защищаемой диссертации**

- (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**, *24* (1), 176. <https://doi.org/10.3390/ijms24010176>
- (2) Boyko, K. M.; **Khrenova, M. G.**; Nikolaeva, A. Y.; Dorovatovskii, P. V.; Vlaskina, A. V.; Subach, O. M.; Popov, V. O.; Subach, F. V. Combined Structural and Computational Study of the mRubyFT Fluorescent Timer Locked in Its Blue Form. *International Journal of Molecular Sciences* **2023**, *24* (9), 7906. <https://doi.org/10.3390/ijms24097906>
- (3) Levina, E. O.; **Khrenova, M. G.**; Tsirelson, V. G. Predicting the Activity of Boronate Inhibitors Against Metallo- β -Lactamase Enzymes. *Supercomputing Frontiers and Innovations* **2022**, *9* (2), 14–32. <https://doi.org/10.14529/jsfi220202>
- (4) Levina, E. O.; **Khrenova, M. G.**; Astakhov, A. A.; Tsirelson, V. G. Keto-Enol Tautomerism from the Electron Delocalization Perspective. *Journal of Computational Chemistry* **2022**, *43* (15), 1000–1010. <https://doi.org/10.1002/jcc.26858>
- (5) Levina, E. O.; **Khrenova, M. G.**; Tsirelson, V. G. The Explicit Role of Electron Exchange in the Hydrogen Bonded Molecular Complexes. *Journal of Computational Chemistry* **2021**, *42* (12), 870–882. <https://doi.org/10.1002/jcc.26507>
- (6) **Khrenova, M. G.**; Levina, E. O.; Tsirelson, V. G. Benchmark Studies of Hydrogen Bond Governing Reactivity of Cephalosporins in L1 Metallo- β -Lactamase: Efficient and Reliable QSPR Equations. *International Journal of Quantum Chemistry* **2021**, *121* (4), e26451. <https://doi.org/10.1002/qua.26451>
- (7) Bartashevich, E. V.; Matveychuk, Y. V.; Mukhitdinova, S. E.; Sobalev, S. A.; **Khrenova, M. G.**; Tsirelson, V. G. The Common Trends for the Halogen, Chalcogen, and Pnictogen Bonds via Sorting Principles and Local Bonding Properties. *Theoretical Chemistry Accounts* **2020**, *139* (2), 26. <https://doi.org/10.1007/s00214-019-2534-y>
- (8) **Khrenova, M. G.**; Tsirelson, V. G. The N \cdots H Hydrogen Bond Strength in the Transition State at the Limiting Step Determines the Reactivity of Cephalosporins in the Active Site of L1 Metallo- β -Lactamase. *Mendeleev Communications* **2019**, *29* (5), 492–494. <https://doi.org/10.1016/j.mencom.2019.09.004>
- (9) **Khrenova, M. G.**; Krivitskaya, A. V.; Tsirelson, V. G. The QM/MM-QTAIM Approach Reveals the Nature of the Different Reactivity of Cephalosporins in the Active Site of L1 Metallo- β -Lactamase. *New Journal of Chemistry* **2019**, *43* (19), 7329–7338. <https://doi.org/10.1039/C9NJ00254E>