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Scientific interests

- 1) The mathematical modelling of immune processes; prediction of immune response with chemoinformatic methods
- 2) Epigenetic changes in obesity and diabetes mellitus
- 3) Statistical criteria of spatiotemporal data clusterisation

Selected Recent Publications

- 1) Smirnov AS, Rudik AV, Filimonov DA, Lagunin AA. TCR-Pred: A new web-application for prediction of epitope and MHC specificity for CDR3 TCR sequences using molecular fragment descriptors. *Immunology*. 2023; 169(4): 447–453. <https://doi.org/10.1111/imm.13641>
- 2) Anton Zadorozhny, Anton Smirnov, Dmitry Filimonov, Alexey Lagunin, Prediction of pathogenic single amino acid substitutions using molecular fragment descriptors, *Bioinformatics*, Volume 39, Issue 8, August 2023, btad484, <https://doi.org/10.1093/bioinformatics/btad484>
- 3) Semeikin, A.V., Fedotcheva, T.A., Sveshnikova, E.D. *et al.* Cytostatic Activity and Ligand-Receptor Interaction Energy of the Novel Russian-Produced Gestagen Gestobutanoil and its Metabolites. *Pharm Chem J* **54**, 1087–1092 (2021). <https://doi.org/10.1007/s11094-021-02326-y>
- 4) Shilov B.V., Smirnov A.S., Savchenko A.Yu. Modeling the interaction of thiozonide and atphase M.tuberculosis by the method of molecular docking. *Journal Biomed.* 2021;17(3E):170-175. (In Russ.) <https://doi.org/10.33647/2713-0428-17-3E-170-175>
- 5) A.M. Pyatnitskiy, V.M. Gukasov, A.S. Smirnov Searching for clusters in population data. *Medicina i vysokie tehnologii*. 2021; №3: 63-71 (In Russ.). <https://doi.org/10.34219/2306-3645-2021-11-3-63-71>