	SHITYAKOV, Sergey V. PhD
Research interests	Neuroscience, precision medicine, bioinformatics, biomedical engineering, and rational drug design at the blood-brain barrier using modern computer modelling methods of chemical interactions
Features of the PhD program	Research results are highly probable to be published in high-impact-factor and peer-reviewed journals, including Nature, Cerebral Cortex, Blood, ACS, and RSC journals.
List of the supervisor's research projects (participation/supervision)	Gazpromneft–Lubricating grant No. A220003100, QSAR modeling for prediction of lubricating oil characteristics, 06/2023–08/2023 (participation)
List of potential thesis topics	✓ Development of virtual screening methods ✓ Creation of virtual libraries ✓ Search for quantitative structure-property relationships (QSAR) of chemical compounds ✓ Experimental verification of QSAR models
Publications in the last five years	46 (Scopus / Web of Science / RSCI)
Key publications	1. Shityakov S., Skorb E., Nosonovsky M. Folding–unfolding asymmetry and a RetroFold computational algorithm//Royal Society Open Science, 2023, Vol. 10, No. 5, pp. 221594 2. Kovalenko A.A., Porozov Y.B., Skorb E.V., Shityakov S. Using novel click chemistry algorithm to design D3R inhibitors as blood-brain barrier permeants//Future Medicinal Chemistry, 2023, Vol. 15, No. 11, pp. 923-935 3. Muravev A.A., Voloshina A.D., Sapunova A.S., Gabdrakhmanova F.B., Lenina O.A., Petrov K.A., Shityakov S., Skorb E.V., Solovieva S.E., Antipin I.S. Calix[4]arene–pyrazole conjugates as potential cancer therapeutics//Bioorganic Chemistry, 2023, Vol. 139, pp. 106742 4. Dutta K., Shityakov S., Maruyama F. DSF inactivator RpfB homologous FadD upregulated in Bradyrhizobium japonicum under iron limiting conditions//Scientific Reports, 2023, Vol. 13, No. 1, pp. 8701

	5. Iwaloye O., Ottu P.O., Olawale F., Babalola O.O., Elekofehinti O.O., Kikiowo B., Adegboyega A.E., Ogbonna H.N., Adeboboye C.F., Folorunso I., Fakayode A.E., Akinjiyan M.O., Onikanni S.A., Shityakov S. Computer-aided drug design in anti-cancer drug discovery: What have we learnt and what is the way forward?//Informatics in Medicine Unlocked, 2023, Vol. 41, pp. 101332
Supervisor's specific requirements	✓ Confident knowledge of programming languages ✓ Work experience with visualization software for complex (bio)molecules
Code of the subject area of the PhD program	1.4.5 Chemoinformatics 1.4.4 Physical Chemistry