

	<p>SHITYAKOV, Sergey V. PhD</p>
<p>Research interests</p>	<p>Neuroscience, precision medicine, bioinformatics, biomedical engineering, and rational drug design at the blood-brain barrier using modern computer modelling methods of chemical interactions</p>
<p>Features of the PhD program</p>	<p>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.</p>
<p>List of the supervisor's research projects (participation/supervision)</p>	<p>Gazpromneft–Lubricating grant No. A220003100, QSAR modeling for prediction of lubricating oil characteristics, 06/2023–08/2023 (participation)</p>
<p>List of potential thesis topics</p>	<ul style="list-style-type: none"> <li>✓ Development of virtual screening methods</li> <li>✓ Creation of virtual libraries</li> <li>✓ Search for quantitative structure-property relationships (QSAR) of chemical compounds</li> <li>✓ Experimental verification of QSAR models</li> </ul>
<p>Publications in the last five years</p>	<p>46 (Scopus / Web of Science / RSCI)</p>
<p>Key publications</p>	<ol style="list-style-type: none"> <li>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</li> <li>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</li> <li>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</li> <li>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</li> </ol>

	<p>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</p>
Supervisor's specific requirements	<ul style="list-style-type: none"> <li>✓ Confident knowledge of programming languages</li> <li>✓ Work experience with visualization software for complex (bio)molecules</li> </ul>
Code of the subject area of the PhD program	<p>1.4.5 Chemoinformatics 1.4.4 Physical Chemistry</p>