

## PERSONAL INFORMATION



## Andrey E Voronkov, PhD

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📅 Date of birth: 19/06/1982

👤 Marital status: married, 2 children

🏠 Residency: Russian Federation – citizen, Norway – permanent resident

RESEARCH FIELDS AND  
PROFESIONAL SKILLS

## Molecular modelling

- Molecular dynamics (software AMBER, GROMACS, NAMD, Desmond) of protein and protein-ligand complexes (tankyrase in complex with small molecule inhibitors, complexes of Frizzled receptors with small molecules), amyloid beta and Frizzled receptors in lipid bilayers, molecular mechanics, homology-based modelling. De novo 3D protein structures modelling (Rosetta), homology-based modelling (Modeller), molecular mechanics methods.

## Chemoinformatics

- QSAR/QSPR model development and usage for activity prediction and virtual screening. Machine-learning methods. Regression analysis, principal component analysis. 3D-QSAR methods: ComFA, CoMSIA, Open3D QSAR.

## Bioinformatics

- Data-mining, big data analysis. Microarray data analysis: expression, genotyping, exon. NGS data analysis: exome, variant calling, RNA Meth-seq. Biostatistics: microarray normalization, regression, multiple test correction. Predictors and clustering analysis of expression data: SVM, KNN, Random Forest, Feature Selection, Cross validation, K-means, SOM, UPGMA. Statistical analysis (t-test, Wilcoxon rank-sum test, Cox regression or Spearman's correlation test).

## Structure-based drug design

- Docking, *de novo* design, scaffold replacement.

## Ligand-based drug design

- Ligand-based screening (ROCS, shape-based etc.). Pharmacophore models construction and pharmacophore-based screening.

## ADME / Tox

- Liver metabolism, adsorption, efflux, toxicity, solubility optimization PC skills (GastroPlus, ADMET predictor, MedChemStudio, different software for CYP metabolism prediction, LogP, PSA and other PK-related properties assessment, modelling and optimization).

Computer usage

- Multiple operational systems and virtual machines, work on cluster with MPI parallel computing applications (MSU Chebyshev, cluster Titan in Oslo), working with distributed volunteer computing (Drugdiscovery@home project).

Medicinal chemistry and organic synthesis

- Medicinal chemistry, organic synthesis retro-synthetic analysis.

Programming

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## MANAGEMENT AND TEACHING SKILLS

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Management. Experience of managing of team of 3 people at Digital BioPharm Ltd. Tasks distribution. Quality control. Multiple collaborations with research groups from academy and industry.

Teaching skills. Supervision of 2 PhD students and 2 MS students at Moscow State University and Moscow Institute of Physics and Technology.

## LANGUAGE SKILLS

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- Russian - native speaker
- English - fluent
- French - proficient
- Norwegian – proficient

## EDUCATION

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- 1999 – 2004 Student, Moscow State University, Department of Chemistry. Moscow, Russian Federation. Specialist diploma.
- 2004 – 2009 PhD student, Moscow State University, Department of Chemistry. Moscow, Russian Federation. PhD thesis defended.

## RESEARCH AND WORK EXPERIENCE

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- 1999 – 2000 Student research project (course project), inorganic chemistry. Moscow, Russian Federation. Inorganic solid-phase synthesis.
- 2000 – 2001 Student research project (course project), analytical chemistry. Moscow, Russian Federation. Different sorts of chromatography, HPLC and others.
- 2001– 2002 Student research project (course project) organic synthesis. Moscow, Russian Federation. 3-step synthesis. Purification. UV, IR spectroscopy.
- 2000 – 2002 Technician in the laboratory, Moscow State University, group of the nucleoproteins, Moscow, Russian Federation
- Telomerase subunits purification research, plasmid genes expression, purification and analysis, TRAP assay

- 2003 – 2004 Master student at Department of Chemistry at Moscow State University, group of molecular modelling and drug design, Moscow, Russian Federation
- Master thesis was devoted to computer modelling of melatonin G-protein coupled receptors and design of their agonists and antagonists
- Sep 2004 - Nov 2010 PhD student, postdoctoral fellow at Department of Chemistry at Moscow State University, group of molecular modelling and drug design, Moscow, Russian Federation
- Computer-assisted drug design. Scientific research during PhD thesis was devoted to modelling of Wnt proteins interactions with Frizzled receptors and design of small molecule regulators for these interactions
  - Scientific supervisor - Dr. Palyulin V.A.
- Nov 2009 -Oct 2013 Postdoctoral fellow at Oslo University Hospital (<http://csc.rr-research.no/?aid=6663&k=cast%2Fgroups>)
- Research in the field of development of small molecule drugs for colorectal cancer treatment. Complex project of drug development and DMPK/ADME/Tox optimization. Interaction with multidisciplinary team of medicinal chemist, organic chemists, cellular and molecular biologists. Patent writing. Scientific papers writing.
  - Scientific supervisor - Prof. Stefan Krauss. Oslo, Norway
- Nov 2013 - Present Founder and Director, Digital BioPharm Ltd., London, UK. Managing team of 3 people. Sales and collaborations setup. Structure-based drug design, ligand-based drug design, ADME/Tox optimization, synthetic and retro-synthetic analysis.
- Dec 2014 - Present Postdoctoral researcher, lecturer, Moscow Institute of Physics and Technology (MIPT) ([www.mipt.ru](http://www.mipt.ru))
- Jun 2014 -Present Postdoctoral researcher, Moscow State University (MSU), Moscow, Russian Federation ([www.msu.ru](http://www.msu.ru))

### OTHER EXPERIENCE

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- 2009-2010 DrugDiscovery@home
- Distributed volunteer computing platform, which relates on volunteer-donated computational time for purposes of drug discovery and modelling computing
  - Research strategy, project idea and strategy development, communication to volunteer developers (Perl, PHP, MySQL, GPU programming)
  - Non-commercial project
  - International, core team in New York, US

### PUBLICATIONS

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- Bhat MA, Al-Omar MA, Ansari MA, Zuheir KM, Imam F, Attia SM, Al-Bakheet SA, Nadeem A, Korashy H, Voronkov A, Berishvili V, Ahmad S. J Med Chem. 2015 Oct 10 [Epub ahead of print]. Design and synthesis of N-aryl-phthalimides as inhibitors of glucocorticoid- induced TNF receptor-related protein, pro-inflammatory mediators, and cytokines in carrageenan-induced lung inflammation. J. Med. Chem., E-pub: 10 October 2015.
- Osolodkin DI, Radchenko EV, Orlov AA, Voronkov AE, Palyulin VA, Zefirov NS. Progress in visual representations of chemical space. Expert Opin Drug Discov. 2015;10(9):959-73.
- Voronkov A., Krauss S. Wnt/beta-catenin signalling and small molecule inhibitors. Curr Pharm Des. 2013;19(4):634-64.
- Waalder J, Machon O, Tumova L, Dinh H, Korinek V, Wilson SR, Paulsen JE, Pedersen NM, Eide TJ, Machonova O, Gradl D, Voronkov A, von Kries JP, Krauss S. A novel tankyrase inhibitor decreases canonical Wnt signaling in colon carcinoma cells and reduces tumor growth in conditional APC mutant mice. Cancer Res. 2012 Jun 1; 72(11):2822-32.
- Voronkov A.E., Baskin I.I., Palyulin V.A., Zefirov N.S. Molecular modelling of modified peptides, potent inhibitors of the xWNT8 and hWNT8 proteins. // J. Mol .Graph. Model., 2008., V. 26., P.1179-1187.
- Voronkov A.E., Baskin I.I., Palyulin V.A., Zefirov N.S. Molecular model of the Wnt protein binding site on the surface of dimeric CRD domain of the hFzd8 receptor. // Dokl. Biochem. Biophys., 2008., V.419., P.75-78.
- Voronkov A.E., Baskin I.I., Palyulin V.A., Zefirov N.S. Molecular modeling of the complex between the xWNT8 protein and the CRD domain of the mFZD8 receptor. // Dokl. Biochem. Biophys., 2007., V.412., P.8-11.
- Voronkov A.E., Ivanov A.A., Baskin I.I., Palyulin V.A., Zefirov N.S. Molecular modeling study of the mechanism of ligand binding to human melatonin receptors. // Dokl. Biochem. Biophys., 2005., V.403., P.284-288.
- Ivanov A.A., Voronkov A.E., Baskin I.I., Palyulin V.A., Zefirov N.S. The study of the mechanism of binding of human ML1A melatonin receptor ligands using molecular modeling. // Dokl. Biochem. Biophys., 2004., V.394., P.49-52.

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All publications overall have more than 150 citations.

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## INTERNATIONAL PATENTS

- Triazole Derivatives As Wnt Signalling Pathway Inhibitors International patent, WO/2012/076898, HOLSWORTH, Daniel, WAALER, Jo, MACHON, Ondrej, KRAUSS, Stefan, VORONKOV, Andrey, GOLDING, Louise. International Application No.:PCT/GB2011/052441, Publication

Date:14.06.2012, International Filing Date: 08.12.2011.

Wnt Pathway Inhibitors International patent WO 2013/093508 A2// HOLSWORTH, Daniel; (US), WAALER, Jo; (NO) ,MACHON, Ondrej; (NO) ,KRAUSS, Stefan; (NO) , VORONKOV, Andrey Edward; International Application, Filing date, 21.12.2013, Priority date 21.12.2013

## REFERENCES

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### **Prof. Stefan Krauss, head of laboratory**

- Section for Cellular and Genetic Therapy
- Institute of Microbiology, Rikshospitalet,
- Sognsvannsveien 9
- 0372, Oslo
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### **Dr. Vladimir A. Palyulin, head of laboratory**

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- Moscow State University:
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### **Dr. Irina Tikhonova, lecturer**

- School of Pharmacy
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### **Dr. Vladimir Chupakhin, researcher**

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