Curriculum vitae: Roman Efremov

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Education

1970–2007	Russia, Moscow	M.V. Lomonosov Moscow State University (biological faculty)	Awarded professor dedree in biophysics
1970–1999	Russia, Moscow	M.V. Lomonosov Moscow State University (biological faculty)	DSc in physics & mathematics; specialization: molecular biophysics (thesis: Molecular modeling of membrane-bound domains of proteins and peptides)
1970–1986	Russia, Moscow	M.V. Lomonosov Moscow State University (biological faculty)	PhD in physics & mathematics (thesis: Topography and microenvironment of chromophore-binding sites in bacterial and visual rhodopsins. Resonance Raman spectroscopy and quantum chemical calculations)
1977–1983	Russia, Moscow	Moscow Engeneering and Physical Institute, Department of Experimental and Theoretical Physics	Ms in biophysics and radiation physics (thesis: «Mathematical algorithms in protein secondary structure determination based on Raman spectroscopic data and prediction techniques»)

IBCh positions

2018–to date	Principal research fellow
2018–to date	Leading research fellow
2021–to date	Deputy sci-director

IBCh memberships

- Educational-methodical commission
- Dissertation council
- Scientific council
- Certifying committee

Titles

- Professor
- Doctor of Science (Physico-mathematical sciences)

Grants and projects

2023–to date	-Молекулярно-биофизическая платформа для изучения мембранных белков: роль олигомеризации и белок-липидных взаимодействий
2018–2022	-Молекулярно-биофизические аспекты олигомеризации мембранных доменов рецепторов, определяющие клеточную сигнализацию в норме и онкогенезе
2018–2021	-
2019–2021	-
2019–2022	Structural biology of membrane proteins for the development of new drugs and diagnostics

Publications

1. Lohan S, Konshina AG, Tiwari RK, **Efremov RG**, Maslennikov I, Parang K (2024). Broad-Spectrum Activity of Membranolytic Cationic Macrocyclic Peptides Against Multi-Drug Resistant Bacteria and Fungi. *Eur J Pharm Sci* 197, 106776, 10.1016/j.ejps.2024.106776
2. El-Mowafi SA, Konshina AG, Mohammed EHM, Krylov NA, **Efremov RG**, Parang K (2023). Structural Analysis and Activity Correlation of Amphiphilic Cyclic Antimicrobial Peptides Derived from the [W4R4] Scaffold. *Molecules* 28 (24), 8049, 10.3390/molecules28248049
3. Mikhnovets IE, Holoubek J, Panina IS, Kotouček J, Gvozdev DA, Chumakov SP, Krasilnikov MS, Zhitlov MY, Gulyak EL, Chistov AA, Nikitin TD, Korshun VA, **Efremov RG**, Alferova VA, Růžek D, Eyer L, Ustinov AV (2023). Alkyl Derivatives of Perylene Photosensitizing Antivirals: Towards Understanding the Influence of Lipophilicity. *Int J Mol Sci* 24 (22), 16483, 10.3390/ijms242216483
4. Aliper ET, **Efremov RG** (2023). Inconspicuous Yet Indispensable: The Coronavirus Spike Transmembrane Domain. *Int J Mol Sci* 24 (22), 16421, 10.3390/ijms242216421
5. Neuberger A, Trofimov YA, Yelshanskaya MV, Khau J, Nadezhdin KD, Khosrof LS, Krylov NA, **Efremov RG**, Sobolevsky AI (2023). Molecular pathway and structural mechanism of human oncochannel TRPV6 inhibition by the phytocannabinoid tetrahydrocannabivarin. *Nat Commun* 14 (1), 4630, 10.1038/s41467-023-40362-2
6. Chugunov AO, Dvoryakova EA, Dyuzheva MA, Simonyan TR, Tereshchenkova VF, Filippova IY, **Efremov RG**, Elpidina EN (2023). Fighting Celiac Disease: Improvement of pH Stability of Cathepsin L In Vitro by Computational Design. *Int J Mol Sci* 24 (15), , 10.3390/ijms241512369
7. Polyansky AA, Gallego LD, **Efremov RG**, Köhler A, Zagrovic B (2023). Protein compactness and interaction valency define the architecture of a biomolecular condensate across scales. *Elife* 12, , 10.7554/eLife.80038
8. Neuberger A, Trofimov YA, Yelshanskaya MV, Nadezhdin KD, Krylov NA, **Efremov RG**, Sobolevsky AI (2023). Structural mechanism of human oncochannel TRPV6 inhibition by the natural phytoestrogen genistein. *Nat Commun* 14 (1), 2659, 10.1038/s41467-023-38352-5
9. Goryacheva E, **Efremov R**, Krylov N, Artemyev I, Bogdanov A, Mamontova A, Pletnev S, Pletneva N, Pletnev V (2023). Crystal Structure of Bright Fluorescent Protein BrUSLEE with Subnanosecond Fluorescence Lifetime; Electric and Dynamic Properties. *Int J Mol Sci* 24 (7), 6403, 10.3390/ijms24076403
10. Bershatsky YV, Kuznetsov AS, Idiatullina AR, Bocharova OV, Dolotova SM, Gavrilenkova AA, Serova OV, Deyev IE, Rakitina TV, Zangieva OT, Pavlov KV, Batishchev OV, Britikov VV, Usanov SA, Arseniev AS, **Efremov RG**, Bocharov EV (2023). Diversity of Structural, Dynamic, and Environmental Effects Explain a Distinctive Functional Role of Transmembrane Domains in the Insulin Receptor Subfamily. *Int J Mol Sci* 24 (4), , 10.3390/ijms24043906
11. Trofimov YA, Minakov AS, Krylov NA, **Efremov RG** (2023). Structural Mechanism of Ionic Conductivity of the TRPV1 Channel. *Dokl Biochem Biophys* 508 (1), 1–5, 10.1134/S1607672922600245
12. Panina IS, Balandin SV, Tsarev AV, Chugunov AO, Tagaev AA, Finkina EI, Antoshina DV, Sheremeteva EV, Paramonov AS, Rickmeyer J, Bierbaum G, **Efremov RG**, Shenkarev ZO, Ovchinnikova TV (2023). Specific Binding of the α-Component of the Lantibiotic Lichenicidin to the Peptidoglycan Precursor Lipid II Predetermines Its Antimicrobial Activity. *Int J Mol Sci* 24 (2), 1332, 10.3390/ijms24021332

13. Polyansky AA, **Efremov RG** (2023). On a mechanistic impact of transmembrane tetramerization in the pathological activation of RTKs. *Comput Struct Biotechnol J* 21, 2837–2844, 10.1016/j.csbj.2023.04.021
14. Lohan S, Konshina AG, **Efremov RG**, Maslennikov I, Parang K (2022). Structure-Based Rational Design of Small α-Helical Peptides with Broad-Spectrum Activity against Multidrug-Resistant Pathogens. *J Med Chem* 66 (1), 855–874, 10.1021/acs.jmedchem.2c01708
15. Goncharuk MV, Baleeva NS, Nolde DE, Gavrikov AS, Mishin AV, Mishin AS, Sosorev AY, Arseniev AS, Goncharuk SA, Borshchevskiy VI, **Efremov RG**, Mineev KS, Baranov MS (2022). Structure-based rational design of an enhanced fluorogen-activating protein for fluorogens based on GFP chromophore. *Commun Biol* 5 (1), 706, 10.1038/s42003-022-03662-9
16. Panina IS, Krylov NA, Chugunov AO, **Efremov RG**, Kordyukova LV (2022). The Mechanism of Selective Recognition of Lipid Substrate by hDHHC20 Enzyme. *Int J Mol Sci* 23 (23), 14791, 10.3390/ijms232314791
17. Gigolaev AM, Lushpa VA, Pinheiro-Junior EL, Tabakmakher VM, Peigneur S, Ignatova AA, Feofanov AV, **Efremov RG**, Mineev KS, Tytgat J, Vassilevski AA (2022). Artificial pore blocker acts specifically on voltage-gated potassium channel isoform KV1.6. *J Biol Chem* 298 (11), 102467, 10.1016/j.jbc.2022.102467
18. Aliper ET, Krylov NA, Nolde DE, Polyansky AA, **Efremov RG** (2022). A Uniquely Stable Trimeric Model of SARS-CoV-2 Spike Transmembrane Domain. *Int J Mol Sci* 23 (16), , 10.3390/ijms23169221
19. Panina I, Krylov N, Gadalla MR, Aliper E, Kordyukova L, Veit M, Chugunov A, **Efremov R** (2022). Molecular Dynamics of DHHC20 Acyltransferase Suggests Principles of Lipid and Protein Substrate Selectivity. *Int J Mol Sci* 23 (9), , 10.3390/ijms23095091
20. Dubovskii PV, Dubova KM, Bourenkov G, Starkov VG, Konshina AG, **Efremov RG**, Utkin YN, Samygina VR (2022). Variability in the Spatial Structure of the Central Loop in Cobra Cytotoxins Revealed by X-ray Analysis and Molecular Modeling. *Toxins (Basel)* 14 (2), , 10.3390/toxins14020149
21. Volynsky P, Maltseva D, Tabakmakher V, Bocharov EV, Raygorodskaya M, Zakharova G, Britikova E, Tonevitsky A, **Efremov R** (2022). Differences in Medium-Induced Conformational Plasticity Presumably Underlie Different Cytotoxic Activity of Ricin and Viscumin. *Biomolecules* 12 (2), , 10.3390/biom12020295
22. Lohan S, Mandal D, Choi W, Konshina AG, Tiwari RK, **Efremov RG**, Maslennikov I, Parang K (2022). Small Amphiphilic Peptides: Activity Against a Broad Range of Drug-Resistant Bacteria and Structural Insight into Membranolytic Properties. *J Med Chem* 65 (1), 665–687, 10.1021/acs.jmedchem.1c01782
23. Bocharov EV, Gremer L, Urban AS, Okhrimenko IS, Volynsky PE, Nadezhdin KD, Bocharova OV, Kornilov DA, Zagryadskaya YA, Kamynina AV, Kuzmichev PK, Kutzsche J, Bolakhrif N, Müller-Schiffmann A, Dencher NA, Arseniev AS, **Efremov RG**, Gordeliy VI, Willbold D (2021). All-d-Enantiomeric Peptide D3 Designed for Alzheimer's Disease Treatment Dynamically Interacts with Membrane-Bound Amyloid-β Precursors. *J Med Chem* 64 (22), 16464–16479, 10.1021/acs.jmedchem.1c00632
24. Panina I, Taldaev A, **Efremov R**, Chugunov A (2021). Molecular dynamics insight into the lipid ii recognition by type a lantibiotics: Nisin, epidermin, and gallidermin. *Micromachines (Basel)* 12 (10), , 10.3390/mi12101169
25. Kulbatskii D, Shenkarev Z, Bychkov M, Loktyushov E, Shulepko M, Koshelev S, Povarov I, Popov A, Peigneur S, Chugunov A, Kozlov S, Sharonova I, **Efremov R**, Skrebitsky V, Tytgat J, Kirpichnikov M, Lyukmanova E (2021). Human Three-Finger Protein Lypd6 Is a Negative Modulator of the Cholinergic System in the Brain. *Front Cell Dev Biol* 9, 662227, 10.3389/fcell.2021.662227
26. Chernykh MA, Kuldyushev NA, Peigneur S, Berkut AA, Tytgat J, **Efremov RG**, Vassilevski AA, Chugunov AO (2021). Derivative of Scorpion Neurotoxin BeM9 Is Selective for Insect Voltage-Gated Sodium Channels. *Russ. J. Bioorganic Chem.* 47 (4), 854–863, 10.1134/S1068162021040063
27. Tabakmakher VM, Gigolaev AM, Peigneur S, Krylov NA, Tytgat J, Chugunov AO, Vassilevski AA, **Efremov RG** (2021). Potassium channel blocker crafted by α-hairpinin scaffold engineering. *Biophys J* 120 (12), 2471–2481, 10.1016/j.bpj.2021.04.020
28. **Efremov RG** (2021). Dynamic "molecular portraits" of biomembranes drawn by their lateral nanoscale inhomogeneities. *Int J Mol Sci* 22 (12), , 10.3390/ijms22126250
29. Tabakmakher VM, Kuzmenkov AI, Gigolaev AM, Pinheiro-Junior EL, Peigneur S, **Efremov RG**, Tytgat J, Vassilevski AA (2021). Artificial Peptide Ligand of Potassium Channel KV1.1 with High Selectivity. *J Evol Biochem Physiol* 57, 386–403, 10.1134/S0022093021020186
30. Krylov NA, **Efremov RG** (2021). libxtc: an efficient library for reading XTC-compressed MD trajectory data.

BMC Res Notes 14 (1), 124, 10.1186/s13104-021-05536-5
31. Konshina AG, Dubovskii PV, **Efremov RG** (2021). Stepwise Insertion of Cobra Cardiotoxin CT2 into a Lipid Bilayer Occurs as an Interplay of Protein and Membrane "Dynamic Molecular Portraits". *J Chem Inf Model* 61 (1), 385–399, 10.1021/acs.jcim.0c01137
32. Nadezhdin KD, Neuberger A, Trofimov YA, Krylov NA, Sinica V, Kupko N, Vlachova V, Zakharian E, **Efremov RG**, Sobolevsky AI (2021). Structural mechanism of heat-induced opening of a temperature-sensitive TRP channel. *Nat Struct Mol Biol* 28 (7), 564–572, 10.1038/s41594-021-00615-4
33. Albrecht C, Kuznetsov AS, Appert-Collin A, Dhaideh Z, Callewaert M, Bershatsky YV, Urban AS, Bocharov EV, Bagnard D, Baud S, Blaise S, Romier-Crouzet B, **Efremov RG**, Dauchez M, Duca L, Gueroult M, Maurice P, Bennasroune A (2020). Transmembrane Peptides as a New Strategy to Inhibit Neuraminidase-1 Activation. *Front Cell Dev Biol* 8, 611121, 10.3389/fcell.2020.611121
34. Kuznetsov AS, Zamaletdinov MF, Bershatsky YV, Urban AS, Bocharova OV, Bennasroune A, Maurice P, Bocharov EV, **Efremov RG** (2020). Dimeric states of transmembrane domains of insulin and IGF-1R receptors: Structures and possible role in activation. *BIOCHIM BIOPHYS ACTA* 1862 (11), 183417, 10.1016/j.bbamem.2020.183417
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37. Gigolaev AM, Kuzmenkov AI, Peigneur S, Tabakmakher VM, Pinheiro-Junior EL, Chugunov AO, **Efremov RG**, Tytgat J, Vassilevski AA (2020). Tuning Scorpion Toxin Selectivity: Switching From KV1.1 to KV1.3. *Front Pharmacol* 11, 1010, 10.3389/fphar.2020.01010
38. Zalygin A, Solovyeva D, Vaskan I, Henry S, Schaefer M, Volynsky P, Tuzikov A, Korchagina E, Ryzhov I, Nizovtsev A, Mochalov K, **Efremov R**, Shtykova E, Oleinikov V, Bovin N (2020). Structure of Supramers Formed by the Amphiphile Biotin-CMG-DOPE. *ChemistryOpen* 9 (6), 640, 10.1002/open.202000139
39. Panina I, Krylov N, Nolde D, **Efremov R**, Chugunov A (2020). Environmental and dynamic effects explain how nisin captures membrane-bound lipid II. *Sci Rep* 10 (1), 8821, 10.1038/s41598-020-65522-y
40. Lubova KI, Chugunov AO, Volynsky PE, Trofimov Y, Korolkova YV, Mosharova IV, Kozlov SA, Andreev YA, **Efremov RG** (2020). Probing temperature and capsaicin-induced activation of TRPV1 channel via computationally guided point mutations in its pore and TRP domains. *Int J Biol Macromol* 158, 1175–1183, 10.1016/j.ijbiomac.2020.04.239
41. Albrecht C, Appert-Collin A, Bagnard D, Blaise S, Romier-Crouzet B, **Efremov RG**, Sartelet H, Duca L, Maurice P, Bennasroune A (2020). Transmembrane Peptides as Inhibitors of Protein-Protein Interactions: An Efficient Strategy to Target Cancer Cells? *Front Oncol* 10, 519, 10.3389/fonc.2020.00519
42. Pakhomov AA, Frolova AY, Tabakmakher VM, Chugunov AO, **Efremov RG**, Martynov VI (2020). Impact of external amino acids on fluorescent protein chromophore biosynthesis revealed by molecular dynamics and mutagenesis studies. *J Photochem Photobiol B* 206, 111853, 10.1016/j.jphotobiol.2020.111853
43. Kudryavtsev DS, Tabakmakher VM, Budylin GS, Egorova NS, **Efremov RG**, Ivanov IA, Belukhina SY, Jegorov AV, Kasheverov IE, Kryukova EV, Shelukhina IV, Shirshin EA, Zhdanova NG, Zhmak MN, Tsetlin VI (2020). Complex approach for analysis of snake venom α-neurotoxins binding to HAP, the high-affinity peptide. *Sci Rep* 10 (1), 3861, 10.1038/s41598-020-60768-y
44. Dubovskii PV, Ignatova AA, Feofanov AV, Utkin YN, **Efremov RG** (2020). Antibacterial activity of cardiotoxin-like basic polypeptide from cobra venom. *Bioorg Med Chem Lett* 30 (3), 126890, 10.1016/j.bmcl.2019.126890
45. Zalygin A, Solovyeva D, Vaskan I, Henry S, Schaefer M, Volynsky P, Tuzikov A, Korchagina E, Ryzhov I, Nizovtsev A, Mochalov K, **Efremov R**, Shtykova E, Oleinikov V, Bovin N (2020). Structure of Supramers Formed by the Amphiphile Biotin-CMG-DOPE. *ChemistryOpen* 9 (6), 641–648, 10.1002/open.201900276
46. Berkut AA, Chugunov AO, Mineev KS, Peigneur S, Tabakmakher VM, Krylov NA, Oparin PB, Lihonosova AF, Novikova EV, Arseniev AS, Grishin EV, Tytgat J, **Efremov RG**, Vassilevski AA (2019). Protein Surface Topography as a tool to enhance the selective activity of a potassium channel blocker. *J Biol Chem* 294 (48),

18349–18359, 10.1074/jbc.RA119.010494
47. Trofimov YA, Krylov NA, **Efremov RG** (2019). Confined Dynamics of Water in Transmembrane Pore of TRPV1 Ion Channel. *Int J Mol Sci* 20 (17), , 10.3390/ijms20174285
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49. Bennasroune A, Romier-Crouzet B, Blaise S, Laffargue M, **Efremov RG**, Martiny L, Maurice P, Duca L (2019). Elastic fibers and elastin receptor complex: Neuraminidase-1 takes the center stage. *Matrix Biol* 84, 57–67, 10.1016/j.matbio.2019.06.007
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51. Polyansky AA, Bocharov EV, Velghe AI, Kuznetsov AS, Bocharova OV, Urban AS, Arseniev AS, Zagrovic B, Demoulin JB, **Efremov RG** (2019). Atomistic mechanism of the constitutive activation of PDGFRA via its transmembrane domain. *BIOCHIM BIOPHYS ACTA* 1863 (1), 82–95, 10.1016/j.bbagen.2018.09.011
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54. Pletneva NV, **Efremov RG**, Goryacheva EA, Artemyev IV, Arkhipova SF, Pletnev VZ (2018). Crystal Structure of the pH-Dependent Green Fluorescent Protein WasCFP with a Tryptophan-Based Chromophore at an Extremely Low pH of 2.0. *Bioorg Khim* 44 (6), 635–639, 10.1134/S0132342318060088
55. Bragin PE, Kuznetsov AS, Bocharova OV, Volynsky PE, Arseniev AS, **Efremov RG**, Mineev KS (2018). Probing the effect of membrane contents on transmembrane protein-protein interaction using solution NMR and computer simulations. *BIOCHIM BIOPHYS ACTA* 1860 (12), 2486–2498, 10.1016/j.bbamem.2018.09.013
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58. Pletneva NV, **Efremov RG**, Goryacheva EA, Artemyev IV, Arkhipova SF, Pletnev VZ (2018). Crystal Structure of the pH-Dependent Green Fluorescent Protein WasCFP with a Tryptophan-Based Chromophore at an Extremely Low pH of 2.0. *Russ. J. Bioorganic Chem.* 44 (6), 640–644, 10.1134/S1068162018060079
59. Panina IS, Chugunov AO, **Efremov RG** (2018). Lipid II as a Target for Novel Antibiotics: Structural and Molecular Dynamics Studies. *Russ. J. Bioorganic Chem.* 44 (6), 653–664, 10.1134/S1068162019010126
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62. Bocharov EV, Lesovoy DM, Bocharova OV, Urban AS, Pavlov KV, Volynsky PE, **Efremov RG**, Arseniev AS (2018). Structural basis of the signal transduction via transmembrane domain of the human growth hormone receptor. *BIOCHIM BIOPHYS ACTA* 1862 (6), 1410–1420, 10.1016/j.bbagen.2018.03.022
63. Крылов НА, Нольде ДЕ, Телегин ПН, **Ефремов РГ**, Шабанов БМ (2018). Производительность современных вычислительных платформ при обработке данных расчетов молекулярной динамики

мембранных и белок-мембранных систем. *Труды НИИСИ РАН* 8 (6), 74–77.
64. **(conference)** Vaskan IS, Solovyeva DO, Chistyakov AA, **Efremov RG**, Volynsky PE, Shtykova EV, Korchagina EYu, Mochalov KE, Bovin NV, Oleinikov VA (2018). Neoglycolipids Micelle-like Structures as a Basis for Drug Delivery Systems. *KnE Energy* 3 (2), 519–527, 10.18502/ken.v3i2.1860
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