

Резюме: Ефремов Роман Гербертович



Адрес

Федеральное государственное
бюджетное учреждение науки
Институт биоорганической химии им.
академиков М.М. Шемякина и Ю.А.
Овчинникова Российской академии
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Контакты

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Образование

1970– 2007	Россия, Москва	Московский государственный университет имени М.В. Ломоносова (МГУ), Биологический факультет	Присвоено ученое звание профессора по специальности «биофизика».
1970– 1999	Россия, Москва	Московский государственный университет имени М.В. Ломоносова (МГУ), Биологический факультет	Диплом доктора физико-математических наук (тема диссертации: «Молекулярное моделирование мембрано- связанных участков белков и пептидов»)
1970– 1986	Россия, Москва	Московский государственный университет имени М.В. Ломоносова (МГУ), Биологический факультет	Диплом кандидата физико-математических наук (тема диссертации: «Топография и микроокружение хромофоров в бактериальном и зрительном родопсинах (спектроскопия комбинационного рассеяния света и квантовохимические расчеты)»)
1977– 1983	Россия, Москва	Московский инженерно- физический институт (МИФИ), Факультет экспериментальной и теоретической физики	Диплом с отличием (тема: «Математические методы определения вторичной структуры белков и полипептидов на основании спектров КР и полуэмпирических расчетов»)

Работа в ИБХ

2018–наст.вр.	Главный научный сотрудник
2018–наст.вр.	Ведущий научный сотрудник
2021–наст.вр.	Заместитель директора по науке

Членство в советах и комиссиях ИБХ

Методическая комиссия
Диссертационный совет
Ученый совет
Аттестационная комиссия

Членство в сообществах

Член редколлегии журналов «Биоорганическая химия», Москва; «The Open Structural Biology Journal», «The Open Bioinformatics Journal».

Член Ученого Совета ИБХ РАН.

Член специализированных диссертационных советов (МГУ, ГУ НИИ БМХ РАН).

Степени и звания

Профессор

Доктор наук (Физико-математические науки, 03.00.02 — Биофизика)

Гранты и проекты

- | | |
|-------------------|--|
| 2023—
наст.вр. | 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 | Управление димеризацией сиалидазы NEU1 как перспективный подход к лечению атеросклероза |
| 2019—
2021 | Динамический «молекулярный портрет» клеточной мембраны и его биологическая роль |
| 2019—
2022 | Структурная биология мембранных белков для создания новых лекарственных и диагностических средств |

Публикации

- 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](#)
- 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](#)
- 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](#)
- Aliper ET, **Efremov RG** (2023). Inconspicuous Yet Indispensable: The Coronavirus Spike Transmembrane Domain. *Int J Mol Sci* 24 (22), 16421, [10.3390/ijms242216421](#)
- 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 tetrahydrocannabinol. *Nat Commun* 14 (1), 4630, [10.1038/s41467-023-40362-2](#)
- 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](#)
- 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](#)
- 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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/10.3389/fcell.2021.662227)
26. Chernykh MA, Kuldyshev 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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/10.1021/acs.jcim.0c01137)
 32. Nadezhdin KD, Neuburger 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](https://doi.org/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](https://doi.org/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](https://doi.org/10.1016/j.bbamem.2020.183417)
 35. Sosorev A, Dominskiy D, Chernyshov I, **Efremov R** (2020). Tuning of Molecular Electrostatic Potential Enables Efficient Charge Transport in Crystalline Azaacenes: A Computational Study. *Int J Mol Sci* 21 (16), 1–18, [10.3390/ijms21165654](https://doi.org/10.3390/ijms21165654)
 36. Belozero OA, Osmakov DI, Vladimirov A, Koshelev SG, Chugunov AO, Andreev YA, Palikov VA, Palikova YA, Shaykhutdinova ER, Gvozd AN, Dyachenko IA, **Efremov RG**, Kublitski VS, Kozlov SA (2020). Sevanol and Its Analogues: Chemical Synthesis, Biological Effects and Molecular Docking. *Pharmaceuticals (Basel)* 13 (8), 1–21, [10.3390/ph13080163](https://doi.org/10.3390/ph13080163)
 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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/10.3390/ijms20174285)
48. Bocharov EV, Nadezhdin KD, Urban AS, Volynsky PE, Pavlov KV, **Efremov RG**, Arseniev AS, Bocharova OV (2019). Familial L723P Mutation Can Shift the Distribution between the Alternative APP Transmembrane Domain Cleavage Cascades by Local Unfolding of the η -Cleavage Site Suggesting a Straightforward Mechanism of Alzheimer's Disease Pathogenesis. *ACS Chem Biol* 14 (7), 1573–1582, [10.1021/acscchembio.9b00309](https://doi.org/10.1021/acscchembio.9b00309)
49. Bennisroune 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](https://doi.org/10.1016/j.matbio.2019.06.007)
50. Tabakmakher VM, Krylov NA, Kuzmenkov AI, **Efremov RG**, Vassilevski AA (2019). Kalium 2.0, a comprehensive database of polypeptide ligands of potassium channels. *Sci Data* 6 (1), 73, [10.1038/s41597-019-0074-x](https://doi.org/10.1038/s41597-019-0074-x)
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](https://doi.org/10.1016/j.bbagen.2018.09.011)
52. Volynsky PE, Nolde DE, Zakharova GS, Palmer RA, Tonevitsky AG, **Efremov RG** (2019). Specific refolding pathway of viscumin A chain in membrane-like medium reveals a possible mechanism of toxin entry into cell. *Sci Rep* 9 (1), 413, [10.1038/s41598-018-36310-6](https://doi.org/10.1038/s41598-018-36310-6)
53. **Efremov RG** (2019). Dielectric-Dependent Strength of Interlipid Hydrogen Bonding in Biomembranes: Model Case Study. *J Chem Inf Model* 59 (6), 2765–2775, [10.1021/acs.jcim.9b00193](https://doi.org/10.1021/acs.jcim.9b00193)
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](https://doi.org/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](https://doi.org/10.1016/j.bbamem.2018.09.013)
56. Kuzmenkov AI, Nekrasova OV, Peigneur S, Tabakmakher VM, Gigolaev AM, Fradkov AF, Kudryashova KS, Chugunov AO, **Efremov RG**, Tytgat J, Feofanov AV, Vassilevski AA (2018). K1.2 channel-specific blocker from Mesobuthus eupeus scorpion venom: Structural basis of selectivity. *Neuropharmacology* 143, 228–238, [10.1016/j.neuropharm.2018.09.030](https://doi.org/10.1016/j.neuropharm.2018.09.030)
57. Dubovskii PV, **Efremov RG** (2018). The role of hydrophobic /hydrophilic balance in the activity of structurally flexible vs rigid cytolytic polypeptides and analogues developed on their basis. *Expert Rev Proteomics* 15 (11), 873–886, [10.1080/14789450.2018.1537786](https://doi.org/10.1080/14789450.2018.1537786)
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](https://doi.org/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](https://doi.org/10.1134/S1068162019010126)
60. Alekseeva AS, Chugunov AO, Volynsky PE, Onishchenko NR, Molotkovsky JG, **Efremov RG**, Boldyrev IA, Vodovozova EL (2018). Behavior of Doxorubicin Lipophilic Conjugates in Liposomal Lipid Bilayers. *Russ. J. Bioorganic Chem.* 44 (6), 732–739, [10.1134/S1068162019010023](https://doi.org/10.1134/S1068162019010023)
61. Dubovskii PV, Ignatova AA, Volynsky PE, Ivanov IA, Zhmak MN, Feofanov AV, **Efremov RG** (2018). Improving therapeutic potential of antibacterial spider venom peptides: coarse-grain molecular dynamics guided approach. *Future Med Chem* 10 (19), 2309–2322, [10.4155/fmc-2018-0170](https://doi.org/10.4155/fmc-2018-0170)
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](https://doi.org/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. (конференция) 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](https://doi.org/10.18502/ken.v3i2.1860)
65. Osmakov DI, Koshelev SG, Andreev YA, Dubinnyi MA, Kublitski VS, **Efremov RG**, Sobolevsky AI, Kozlov SA (2018). Proton-independent activation of acid-sensing ion channel 3 by an alkaloid, lindoldhamine, from *Laurus nobilis*. *Br J Pharmacol* 175 (6), 924–937, [10.1111/bph.14134](https://doi.org/10.1111/bph.14134)
66. Konshina AG, Krylov NA, **Efremov RG** (2017). Cardiotoxins: Functional Role of Local Conformational Changes. *J Chem Inf Model* 57 (11), 2799–2810, [10.1021/acs.jcim.7b00395](https://doi.org/10.1021/acs.jcim.7b00395)
67. (конференция) Kuznetsov AS, Smirnov KV, Antonov MY, Nikolaev IN, **Efremov RG** (2017). Molecular modeling of biomembranes and their complexes with protein transmembrane α -helices. *AIP Conf Proc* 1907, , [10.1063/1.5012645](https://doi.org/10.1063/1.5012645)
68. Dubovskii PV, Dubinnyi MA, Volynsky PE, Pustovalova YE, Konshina AG, Utkin YN, Arseniev AS, **Efremov RG** (2017). Impact of membrane partitioning on the spatial structure of an S-type cobra cytotoxin. *J Biomol Struct Dyn* 36 (13), 1–16, [10.1080/07391102.2017.1389662](https://doi.org/10.1080/07391102.2017.1389662)
69. Нольде ДЕ, Крылов НА, Телегин ПН, **Ефремов РГ**, Шабанов БМ (2017). Производительность современных вычислительных платформ в расчетах молекулярной динамики белок - мембранных систем. *Труды НИИСИ РАН* 7 (4), 157–161.
70. Volynsky P, **Efremov R**, Mikhalev I, Dobrochaeva K, Tuzikov A, Korchagina E, Obukhova P, Rapoport E, Bovin N (2017). Why human anti-Gal α 1–4Gal β 1–4Glc natural antibodies do not recognize the trisaccharide on erythrocyte membrane? Molecular dynamics and immunochemical investigation. *Mol Immunol* 90, 87–97, [10.1016/j.molimm.2017.06.247](https://doi.org/10.1016/j.molimm.2017.06.247)
71. Dubovskii PV, Dubinnyi MA, Konshina AG, Kazakova ED, Sorokoumova GM, Ilyasova TM, Shulepko MA, Chertkova RV, Lyukmanova EN, Dolgikh DA, Arseniev AS, **Efremov RG** (2017). Structural and Dynamic Portraits of Recombinant and Native Cytotoxin I from *Naja oxiana*: How Close Are They? *Biochemistry* 56 (34), 4468–4477, [10.1021/acs.biochem.7b00453](https://doi.org/10.1021/acs.biochem.7b00453)
72. Kuzmenkov AI, Peigneur S, Chugunov AO, Tabakmakher VM, **Efremov RG**, Tytgat J, Grishin EV, Vassilevski AA (2017). C-Terminal residues in small potassium channel blockers OdK1 and OSK3 from scorpion venom fine-tune the selectivity. *BIOCHIM BIOPHYS ACTA* 1865 (5), 465–472, [10.1016/j.bbapap.2017.02.001](https://doi.org/10.1016/j.bbapap.2017.02.001)
73. Bocharov EV, Mineev KS, Pavlov KV, Akimov SA, Kuznetsov AS, **Efremov RG**, Arseniev AS (2017). Helix-helix interactions in membrane domains of bitopic proteins: Specificity and role of lipid environment. *BIOCHIM BIOPHYS ACTA* 1859 (4), 561–576, [10.1016/j.bbamem.2016.10.024](https://doi.org/10.1016/j.bbamem.2016.10.024)
74. Bocharov EV, Bragin PE, Pavlov KV, Bocharova OV, Mineev KS, Polyansky AA, Volynsky PE, **Efremov RG**, Arseniev AS (2017). The Conformation of the Epidermal Growth Factor Receptor Transmembrane Domain Dimer Dynamically Adapts to the Local Membrane Environment. *Biochemistry* 56 (12), 1697–1705, [10.1021/acs.biochem.6b01085](https://doi.org/10.1021/acs.biochem.6b01085)
75. (книга) Kuznetsov AS, Volynsky PE, **Efremov RG** (2017). A molecular basis of protein-protein interactions in

membranes: A computational investigation. , 89–108.

76. (книга) Pyrkova DV, **Efremov RG** (2017). The structural and dynamic properties of lipid bilayers exhibit concordant changes: MD simulations. , 73–88.
77. Maurice P, Baud S, Bocharova OV, Bocharov EV, Kuznetsov AS, Kawecki C, Bocquet O, Romier B, Gorisse L, Ghirardi M, Duca L, Blaise S, Martiny L, Dauchez M, **Efremov RG**, Debelle L (2016). New Insights into Molecular Organization of Human Neuraminidase-1: Transmembrane Topology and Dimerization Ability. *Sci Rep* 6, 38363, [10.1038/srep38363](https://doi.org/10.1038/srep38363)
78. Kasheverov IE, Chugunov AO, Kudryavtsev DS, Ivanov IA, Zhmak MN, Shelukhina IV, Spirova EN, Tabakmakher VM, Zelepuga EA, **Efremov RG**, Tsetlin VI (2016). High-Affinity α -Conotoxin PnIA Analogs Designed on the Basis of the Protein Surface Topography Method. *Sci Rep* 6, 36848, [10.1038/srep36848](https://doi.org/10.1038/srep36848)
79. Плетнёв ВЗ, Плетнева НВ, **Ефремов РГ**, Горячева ЕА, Артемьев ИВ, Архипова СФ, Саркисян КС, Мишин АС, Лукьянов КА, Плетнев СВ (2016). Пространственная структура pH-зависимого зеленого флуоресцентного белка WASCFP с депротонированным хромофором на основе триптофана. 42 (6), 675–682.
80. Pletnev VZ, Pletneva NV, **Efremov RG**, Goryacheva EA, Artemyev IV, Arkhipova SF, Sarkisyan KS, Mishin AS, Lukyanov KA, Pletnev SV (2016). Three-dimensional structure of a pH-dependent fluorescent protein WasCFP with a tryptophan based deprotonated chromophore. *Russ. J. Bioorganic Chem.* 42 (6), 612–618, [10.1134/S1068162016050149](https://doi.org/10.1134/S1068162016050149)
81. (конференция) Панина ИС, Нольде ДЕ, Чугунов АО, **Ефремов РГ** (2016). Структурно-динамическая модель комплекса лантибиотика низин с липидом-II в биомембране. 1, 263–267.
82. Chugunov AO, Volynsky PE, Krylov NA, Nolde DE, **Efremov RG** (2016). Temperature-sensitive gating of TRPV1 channel as probed by atomistic simulations of its trans- and juxtamembrane domains. *Sci Rep* 6, 33112, [10.1038/srep33112](https://doi.org/10.1038/srep33112)
83. Lyukmanova EN, Shulepko MA, Shenkarev ZO, Kasheverov IE, Chugunov AO, Kulbatskii DS, Myshkin MY, Utkin YN, **Efremov RG**, Tsetlin VI, Arseniev AS, Kirpichnikov MP, Dolgikh DA (2016). Central loop of non-conventional toxin WTX from *Naja kaouthia* is important for interaction with nicotinic acetylcholine receptors. *Toxicon* 119, 274–279, [10.1016/j.toxicon.2016.06.012](https://doi.org/10.1016/j.toxicon.2016.06.012)
84. Lyukmanova EN, Shulepko MA, Shenkarev ZO, Bychkov ML, Paramonov AS, Chugunov AO, Kulbatskii DS, Arvaniti M, Dolejsi E, Schaer T, Arseniev AS, **Efremov RG**, Thomsen MS, Dolezal V, Bertrand D, Dolgikh DA, Kirpichnikov MP (2016). Secreted Isoform of Human Lynx1 (SLURP-2): Spatial Structure and Pharmacology of Interactions with Different Types of Acetylcholine Receptors. *Sci Rep* 6, 30698, [10.1038/srep30698](https://doi.org/10.1038/srep30698)
85. (конференция) Кузнецов АС, **Ефремов РГ** (2016). Оценка влияния среды на димеризацию трансмембранных доменов гликофорина А в компьютерном эксперименте. 1 (1), 250–254.
86. Kuznetsov AS, Volynsky PE, **Efremov RG** (2015). Role of the lipid environment in the dimerization of transmembrane domains of glycoporphin A. *Acta Naturae* 7 (4), 122–127, [10.32607/20758251-2015-7-4-122-127](https://doi.org/10.32607/20758251-2015-7-4-122-127)
87. Lyukmanova EN, Shenkarev ZO, Shulepko MA, Paramonov AS, Chugunov AO, Janickova H, Dolejsi E, Dolezal V, Utkin YN, Tsetlin VI, Arseniev AS, **Efremov RG**, Dolgikh DA, Kirpichnikov MP (2015). Structural insight into specificity of interactions between nonconventional three-finger weak toxin from *Naja kaouthia* (WTX) and muscarinic acetylcholine receptors. *J Biol Chem* 290 (39), 23616–23630, [10.1074/jbc.M115.656595](https://doi.org/10.1074/jbc.M115.656595)
88. Kuznetsov AS, Polyansky AA, Fleck M, Volynsky PE, **Efremov RG** (2015). Adaptable Lipid Matrix Promotes Protein-Protein Association in Membranes. *J Chem Theory Comput* 11 (9), 4415–4426, [10.1021/acs.jctc.5b00206](https://doi.org/10.1021/acs.jctc.5b00206)
89. Dubovskii PV, Vassilevski AA, Kozlov SA, Feofanov AV, Grishin EV, **Efremov RG** (2015). Latarecins: Versatile spider venom peptides. *Cell Mol Life Sci* 72 (23), 4501–4522, [10.1007/s00018-015-2016-x](https://doi.org/10.1007/s00018-015-2016-x)
90. Kasheverov IE, Kudryavtsev DS, Ivanov IA, Zhmak MN, Chugunov AO, Tabakmakher VM, Zelepuga EA, **Efremov RG**, Tsetlin VI (2015). Rational design of new ligands for nicotinic receptors on the basis of α -conotoxin PnIA. *Dokl Biochem Biophys* 461 (1), 106–109, [10.1134/S1607672915020118](https://doi.org/10.1134/S1607672915020118)
91. Dubovskii PV, Vorontsova OV, Utkin YN, Arseniev AS, **Efremov RG**, Feofanov AV (2015). Cobra cytotoxins: Determinants of antibacterial activity. *MENDELEEV COMMUN* 25 (1), 70–71, [10.1016/j.mencom.2015.01.026](https://doi.org/10.1016/j.mencom.2015.01.026)
92. Kuznetsov AS, Polyansky AA, Volynsky PE, **Efremov RG** (2015). Lipid environment promotes dimerization of

transmembrane helices. , 139–150.

93. Chugunov AO, Volynsky PE, Krylov NA, Boldyrev IA, **Efremov RG** (2014). Liquid but durable: Molecular dynamics simulations explain the unique properties of archaeal-like membranes. *Sci Rep* 4, 7462, [10.1038/srep07462](https://doi.org/10.1038/srep07462)
94. Чугунов АО, **Ефремов РГ** (2014). Поверхность молекулы -- источник биологической информации. (10), 3–10.
95. Кузнецов АС, Дубовский ПВ, Воронцова ОВ, Фефанов АВ, **Ефремов РГ** (2014). Взаимодействие линейных катионных пептидов с фосфолипидными мембранами и полимерами сиаловой кислоты. *Biochemistry (Mosc)* 79 (5), 583–594.
96. Polyansky AA, Chugunov AO, Volynsky PE, Krylov NA, Nolde DE, **Efremov RG** (2014). PREDDIMER: A web server for prediction of transmembrane helical dimers. *Bioinformatics* 30 (6), 889–890, [10.1093/bioinformatics/btt645](https://doi.org/10.1093/bioinformatics/btt645)
97. Kuznetsov AS, Dubovskii PV, Vorontsova OV, Feofanov AV, **Efremov RG** (2014). Interaction of linear cationic peptides with phospholipid membranes and polymers of sialic acid. *Biochemistry (Mosc)* 79 (5), 459–468, [10.1134/S0006297914050101](https://doi.org/10.1134/S0006297914050101)
98. Malakhov MV, Dubinnyi MA, Vlasova NV, Zgoda VG, **Efremov RG**, Boldyrev IA (2014). End-group differentiating ozonolysis of furocoumarins. *RSC Adv* 4 (106), 61277–61280, [10.1039/c4ra08106d](https://doi.org/10.1039/c4ra08106d)
99. Dubovskii PV, Konshina AG, **Efremov RG** (2014). Cobra cardiotoxins: Membrane interactions and pharmacological potential. *Curr Med Chem* 21 (3), 270–287, [10.2174/09298673113206660315](https://doi.org/10.2174/09298673113206660315)
100. Koromyslova AD, Chugunov AO, **Efremov RG** (2014). Deciphering fine molecular details of proteins' structure and function with a protein surface topography (PST) method. *J Chem Inf Model* 54 (4), 1189–1199, [10.1021/ci500158y](https://doi.org/10.1021/ci500158y)
101. Kuznetsov AS, Volynsky PE, **Efremov RG** (2013). Probing free energy of transmembrane helix-helix association via a novel single-residue based approach. , 97–108.
102. Krylov NA, Pentkovsky VM, **Efremov RG** (2013). Nontrivial behavior of water in the vicinity and inside lipid bilayers as probed by molecular dynamics simulations. *ACS Nano* 7 (10), 9428–9442, [10.1021/nn4042392](https://doi.org/10.1021/nn4042392)
103. Chugunov AO, Koromyslova AD, Berkut AA, Peigneur S, Tytgat J, Polyansky AA, Pentkovsky VM, Vassilevski AA, Grishin EV, **Efremov RG** (2013). Modular organization of α -toxins from scorpion venom mirrors domain structure of their targets, sodium channels. *J Biol Chem* 288 (26), 19014–19027, [10.1074/jbc.M112.431650](https://doi.org/10.1074/jbc.M112.431650)
104. Volynsky PE, Polyansky AA, Fakhrutdinova GN, Bocharov EV, **Efremov RG** (2013). Role of dimerization efficiency of transmembrane domains in activation of fibroblast growth factor receptor 3. *J Am Chem Soc* 135 (22), 8105–8108, [10.1021/ja4011942](https://doi.org/10.1021/ja4011942)
105. Chugunov A, Pyrkova D, Nolde D, Polyansky A, Pentkovsky V, **Efremov R** (2013). Lipid-II forms potential "landing terrain" for lantibiotics in simulated bacterial membrane. *Sci Rep* 3, 1678, [10.1038/srep01678](https://doi.org/10.1038/srep01678)
106. Blanchevove C, Floquet N, Scandolera A, Baud S, Maurice P, Bocquet O, Blaise S, Ghoneim C, Cantarelli B, Delacoux F, Dauchez M, **Efremov RG**, Martiny L, Duca L, Debelle L (2013). Interaction between the elastin peptide VGVAPG and human elastin binding protein. *J Biol Chem* 288 (2), 1317–1328, [10.1074/jbc.M112.419929](https://doi.org/10.1074/jbc.M112.419929)
107. Чугунов АО, Нольде ДЕ, Пыркова ДВ, Полянский АА, Пентковский ВМ, **Ефремов РГ** (2013). На пути к новым антибиотикам. 12, 34–36.
108. Чугунов АО, Полянский АА, **Ефремов РГ** (2013). Физическая водобоязнь. 1, 24–34.
109. Aseev LV, Chugunov AO, **Efremov RG**, Boni IV (2013). A single missense mutation in a coiled-coil domain of Escherichia coli ribosomal protein S2 confers a thermosensitive phenotype that can be suppressed by ribosomal protein S1. *J Bacteriol* 195 (1), 95–104, [10.1128/JB.01305-12](https://doi.org/10.1128/JB.01305-12)
110. Pyrkova DV, Tarasova NK, Krylov NA, Nolde DE, Pentkovsky VM, **Efremov RG** (2013). Dynamic clustering of lipids in hydrated two-component membranes: Results of computer modeling and putative biological impact. *J Biomol Struct Dyn* 31 (1), 87–95, [10.1080/07391102.2012.691365](https://doi.org/10.1080/07391102.2012.691365)
111. Pyrkova DV, Tarasova NK, Krylov NA, Nolde DE, **Efremov RG** (2013). Lateral heterogeneity as an intrinsic property of hydrated lipid bilayers: A molecular dynamics study. , 85–101.
112. Konshina AG, Dubovskii PV, **Efremov RG** (2012). Structure and dynamics of cardiotoxins. *Curr Protein Pept Sci* 13 (6), 570–584, [10.2174/138920312803582960](https://doi.org/10.2174/138920312803582960)

113. Polyansky AA, Chugunov AO, Vassilevski AA, Grishin EV, **Efremov RG** (2012). Recent advances in computational modeling of α -Helical membrane-active peptides. *Curr Protein Pept Sci* 13 (7), 644–657, [10.2174/138920312804142147](https://doi.org/10.2174/138920312804142147)
114. Charlier L, Topin J, Ronin C, Kim SK, Goddard WA, **Efremov R**, Golebiowski J (2012). How broadly tuned olfactory receptors equally recognize their agonists. Human OR1G1 as a test case. *Cell Mol Life Sci* 69 (24), 4205–4213, [10.1007/s00018-012-1116-0](https://doi.org/10.1007/s00018-012-1116-0)
115. Polyansky AA, Volynsky PE, **Efremov RG** (2012). Multistate organization of transmembrane helical protein dimers governed by the host membrane. *J Am Chem Soc* 134 (35), 14390–14400, [10.1021/ja303483k](https://doi.org/10.1021/ja303483k)
116. Ostapchenko VG, Gasparian ME, Kosinsky YA, **Efremov RG**, Dolgikh DA, Kirpichnikov MP (2012). Dissecting structural basis of the unique substrate selectivity of human enteropeptidase catalytic subunit. *J Biomol Struct Dyn* 30 (1), 62–73, [10.1080/07391102.2012.674249](https://doi.org/10.1080/07391102.2012.674249)
117. Чугунов АО, Полянский АА, **Ефремов РГ** (2012). Липидный фундамент жизни. (3), 3–12.
118. Pyrkova DV, Tarasova NK, Krylov NA, Nolde DE, **Efremov RG** (2012). Lateral heterogeneity as an intrinsic property of hydrated lipid bilayers: A molecular dynamics study. , 85–101.
119. **(книга) Efremov RG**, Chugunov AO, Pyrkov TV, Priestle JP, Pentkovsky VM, Arseniev AS, Jacoby E (2012). Molecular Lipophilicity in Protein Modeling and Drug Design. *Frontiers in Drug Design and Discovery* 6, 249–290, [10.2174/9781608054640113060013](https://doi.org/10.2174/9781608054640113060013)
120. Pyrkova DV, Tarasova NK, Krylov NA, Nolde DE, **Efremov RG** (2011). Lateral clustering of lipids in hydrated bilayers composed of dioleoylphosphatidylcholine and dipalmitoylphosphatidylcholine. *BIOL MEMBRANY* 28 (4), 298–306.
121. Pyrkova DV, Tarasova NK, Krylov NA, Nolde DE, **Efremov RG** (2011). Lateral clustering of lipids in hydrated bilayers composed of dioleoylphosphatidylcholine and dipalmitoylphosphatidylcholine. *Biochem (Mosc) Suppl Ser A Membr Cell Biol* 5 (3), 278–285, [10.1134/S1990747811040106](https://doi.org/10.1134/S1990747811040106)
122. **(конференция) Lesovoy DM**, Bocharov EV, Mayzel ML, Goncharuk SA, Goncharuk MV, Volynsky PE, **Efremov RG**, Arseniev AS (2011). Structural and dynamical model of transmembrane domain of fibroblast growth factor receptor 3. *EUROMAR 2011* , 191.
123. Kordyukova LV, Serebryakova MV, Polyansky AA, Kropotkina EA, Alexeevski AV, Veit M, **Efremov RG**, Filippova IY, Baratova LA (2011). Linker and/or transmembrane regions of influenza A/Group-1, A/Group-2, and type B virus hemagglutinins are packed differently within trimers. *BIOCHIM BIOPHYS ACTA* 1808 (7), 1843–1854, [10.1016/j.bbamem.2011.03.005](https://doi.org/10.1016/j.bbamem.2011.03.005)
124. Deyev IE, Sohet F, Vassilenko KP, Serova OV, Popova NV, Zozulya SA, Burova EB, Houillier P, Rzhnevsky DI, Berchatova AA, Murashev AN, Chugunov AO, **Efremov RG**, Nikol'sky NN, Bertelli E, Eladari D, Petrenko AG (2011). Insulin receptor-related receptor as an extracellular alkali sensor. *Cell Metab* 13 (6), 679–689, [10.1016/j.cmet.2011.03.022](https://doi.org/10.1016/j.cmet.2011.03.022)
125. Polyansky AA, Volynsky PE, **Efremov RG** (2011). Structural, dynamic, and functional aspects of helix association in membranes: A computational view. *Adv Protein Chem Struct Biol* 83, 129–161, [10.1016/B978-0-12-381262-9.00004-5](https://doi.org/10.1016/B978-0-12-381262-9.00004-5)
126. Konshina AG, Boldyrev IA, Utkin YN, Omelkov AV, **Efremov RG** (2011). Snake cytotoxins bind to membranes via interactions with phosphatidylserine head groups of lipids. *PLoS One* 6 (4), e19064, [10.1371/journal.pone.0019064](https://doi.org/10.1371/journal.pone.0019064)
127. Mineev KS, Bocharov EV, Volynsky PE, Goncharuk MV, Tkach EN, Ermolyuk YS, Schulga AA, Chupin VV, Maslennikov IV, **Efremov RG**, Arseniev AS (2011). Dimeric structure of the transmembrane domain of glycophorin a in lipidic and detergent environments. *Acta Naturae* 3 (2), 90–8.
128. Pyrkova DV, Tarasova NK, Pyrkov TV, Krylov NA, **Efremov RG** (2011). Atomic-scale lateral heterogeneity and dynamics of two-component lipid bilayers composed of saturated and unsaturated phosphatidylcholines. *Soft Matter* 7 (6), 2569–2579, [10.1039/c0sm00701c](https://doi.org/10.1039/c0sm00701c)
129. Чугунов АО, **Ефремов РГ** (2010). Компьютерные игры в молекулярную биофизику. (12), 36–43.
130. Polyansky AA, Ramaswamy R, Volynsky PE, Sbalzarini IF, Marrink SJ, **Efremov RG** (2010). Antimicrobial peptides induce growth of phosphatidylglycerol domains in a model bacterial membrane. *J Phys Chem Lett* 1 (20), 3108–3111, [10.1021/jz101163e](https://doi.org/10.1021/jz101163e)
131. Konshina AG, Boldyrev IA, Omelkov AV, Utkin YN, **Efremov RG** (2010). Anionic lipids: determinants of binding cytotoxins from snake venom on the surface of cell membranes. *Acta Naturae* 2 (2), 88–96.

132. Pyrkov TV, Ozerov IV, Balitskaya ED, **Efremov RG** (2010). Molecular docking: The role of noncovalent interactions in the formation of protein-nucleotide and protein-peptide complexes. *Russ. J. Bioorganic Chem.* 36 (4), 446–455, [10.1134/S1068162010040023](https://doi.org/10.1134/S1068162010040023)
133. Novoseletsky VN, Pyrkov TV, **Efremov RG** (2010). Analysis of hydrophobic interactions of antagonists with the beta2-adrenergic receptor. *SAR QSAR Environ Res* 21 (12), 37–55, [10.1080/10629360903560637](https://doi.org/10.1080/10629360903560637)
134. Bocharov EV, Mayzel ML, Volynsky PE, Mineev KS, Tkach EN, Ermolyuk YS, Schulga AA, **Efremov RG**, Arseniev AS (2010). Left-handed dimer of EphA2 transmembrane domain: Helix packing diversity among receptor tyrosine kinases. *Biophys J* 98 (5), 881–889, [10.1016/j.bpj.2009.11.008](https://doi.org/10.1016/j.bpj.2009.11.008)
135. Lashkov AA, Zhukhlistova NE, Gabdoulkhakov AH, Shtil AA, **Efremov RG**, Betzel C, Mikhailov AM (2010). The X-ray structure of Salmonella typhimurium uridine nucleoside phosphorylase complexed with 2,2'-anhydrouridine, phosphate and potassium ions at 1.86 Å resolution. *Acta Crystallogr D Biol Crystallogr* 66 (1), 51–60, [10.1107/S0907444909044175](https://doi.org/10.1107/S0907444909044175)
136. Bocharov EV, Volynsky PE, Pavlov KV, **Efremov RG**, Arseniev AS (2010). Structure elucidation of dimeric transmembrane domains of bitopic proteins. *Cell Adh Migr* 4 (2), 284–298, [10.4161/cam.4.2.11930](https://doi.org/10.4161/cam.4.2.11930)
137. Volynsky PE, Mineeva EA, Goncharuk MV, Ermolyuk YS, Arseniev AS, **Efremov RG** (2010). Computer simulations and modeling-assisted ToxR screening in deciphering 3D structures of transmembrane α -helical dimers: Ephrin receptor A1. *Phys Biol* 7 (1), 16014, [10.1088/1478-3975/7/1/016014](https://doi.org/10.1088/1478-3975/7/1/016014)
138. Pyrkov TV, Chugunov AO, Krylov NA, Nolde DE, **Efremov RG** (2009). Complementarity of hydrophobic/hydrophilic properties in protein-ligand complexes: A new tool to improve docking results. *Vierteljahrschr Soz Wirtschaftsgesch* 28 (1), 21–41, [10.1007/978-90-481-2368-1_2](https://doi.org/10.1007/978-90-481-2368-1_2)
139. Чугунов АО, **Ефремов РГ** (2009). Предсказание пространственной структуры белков: акцент на мембранных мишенях. 35 (6), 1–17.
140. Chugunov AO, **Efremov RG** (2009). Prediction of the spatial structure of proteins: emphasis on membrane targets. *Bioorg Khim* 35 (6), 744–760.
141. Chugunov AO, **Efremov RG** (2009). Prediction of the spatial structure of proteins: Emphasis on membrane targets. *Russ. J. Bioorganic Chem.* 35 (6), 670–684, [10.1134/S106816200906003X](https://doi.org/10.1134/S106816200906003X)
142. Lesovoy DM, Bocharov EV, Lyukmanova EN, Kosinsky YA, Shulepko MA, Dolgikh DA, Kirpichnikov MP, **Efremov RG**, Arseniev AS (2009). Specific membrane binding of neurotoxin II can facilitate its delivery to acetylcholine receptor. *Biophys J* 97 (7), 2089–2097, [10.1016/j.bpj.2009.07.037](https://doi.org/10.1016/j.bpj.2009.07.037)
143. Polyansky AA, Vassilevski AA, Volynsky PE, Vorontsova OV, Samsonova OV, Egorova NS, Krylov NA, Feofanov AV, Arseniev AS, Grishin EV, **Efremov RG** (2009). N-terminal amphipathic helix as a trigger of hemolytic activity in antimicrobial peptides: A case study in laticins. *FEBS Lett* 583 (14), 2425–2428, [10.1016/j.febslet.2009.06.044](https://doi.org/10.1016/j.febslet.2009.06.044)
144. Pyrkov TV, Chugunov AO, Krylov NA, Nolde DE, **Efremov RG** (2009). PLATINUM: A web tool for analysis of hydrophobic/hydrophilic organization of biomolecular complexes. *Bioinformatics* 25 (9), 1201–1202, [10.1093/bioinformatics/btp111](https://doi.org/10.1093/bioinformatics/btp111)
145. Pyrkov TV, Pyrkova DV, Balitskaya ED, **Efremov RG** (2009). The role of stacking interactions in complexes of proteins with adenine and Guanine fragments of ligands. *Acta Naturae* 1 (1), 124–7.
146. Polyansky AA, Volynsky PE, Arseniev AS, **Efremov RG** (2009). Adaptation of a membrane-active peptide to heterogeneous environment. II. The role of mosaic nature of the membrane surface. *J Phys Chem B* 113 (4), 1120–1126, [10.1021/jp803641x](https://doi.org/10.1021/jp803641x)
147. Polyansky AA, Volynsky PE, Arseniev AS, **Efremov RG** (2009). Adaptation of a membrane-active peptide to heterogeneous environment. I. Structural plasticity of the peptide. *J Phys Chem B* 113 (4), 1107–1119, [10.1021/jp803640e](https://doi.org/10.1021/jp803640e)
148. Bocharov EV, Mayzel ML, Volynsky PE, Goncharuk MV, Ermolyuk YS, Schulga AA, Artemenko EO, **Efremov RG**, Arseniev AS (2008). Spatial structure and pH-dependent conformational diversity of dimeric transmembrane domain of the receptor tyrosine kinase EphA1. *J Biol Chem* 283 (43), 29385–29395, [10.1074/jbc.M803089200](https://doi.org/10.1074/jbc.M803089200)
149. Farce A, Chugunov AO, Logé C, Sabaouni A, Yous S, Dilly S, Renault N, Vergoten G, **Efremov RG**, Lesieur D, Chavatte P (2008). Homology modeling of MT1 and MT2 receptors. *Eur J Med Chem* 43 (9), 1926–1944, [10.1016/j.ejmech.2007.12.001](https://doi.org/10.1016/j.ejmech.2007.12.001)
150. Dubovskii PV, Volynsky PE, Polyansky AA, Karpunin DV, Chupin VV, **Efremov RG**, Arseniev AS (2008).

Three-dimensional structure/hydrophobicity of laticins specifies their mode of membrane activity.

Biochemistry 47 (11), 3525–3533, [10.1021/bi702203w](https://doi.org/10.1021/bi702203w)

151. Bocharov EV, Mineev KS, Volynsky PE, Ermolyuk YS, Tkach EN, Sobol AG, Chupin VV, Kirpichnikov MP, **Efremov RG**, Arseniev AS (2008). Spatial structure of the dimeric transmembrane domain of the growth factor receptor ErbB2 presumably corresponding to the receptor active state. *J Biol Chem* 283 (11), 6950–6956, [10.1074/jbc.M709202200](https://doi.org/10.1074/jbc.M709202200)
152. Pyrkov TV, Priestle JP, Jacoby E, **Efremov RG** (2008). Ligand-specific scoring functions: Improved ranking of docking solutions. *SAR QSAR Environ Res* 19 (12), 91–99, [10.1080/10629360701844092](https://doi.org/10.1080/10629360701844092)
153. Vereshaga YA, Volynsky PE, Pustovalova JE, Nolde DE, Arseniev AS, **Efremov RG** (2007). Specificity of helix packing in transmembrane dimer of the cell death factor BNIP3: A molecular modeling study. *Proteins* 69 (2), 309–325, [10.1002/prot.21555](https://doi.org/10.1002/prot.21555)
154. Pyrkov TV, **Efremov RG** (2007). A fragment-based scoring function to re-rank ATP docking results. *Int J Mol Sci* 8 (11), 1083–1094, [10.3390/i8111083](https://doi.org/10.3390/i8111083)
155. Bocharov EV, Pustovalova YE, Pavlov KV, Volynsky PE, Goncharuk MV, Ermolyuk YS, Karpunin DV, Schulga AA, Kirpichnikov MP, **Efremov RG**, Maslennikov IV, Arseniev AS (2007). Unique dimeric structure of BNIP3 transmembrane domain suggests membrane permeabilization as a cell death trigger. *J Biol Chem* 282 (22), 16256–16266, [10.1074/jbc.M701745200](https://doi.org/10.1074/jbc.M701745200)
156. Pyrkov TV, Kosinsky YA, Arseniev AS, Priestle JP, Jacoby E, **Efremov RG** (2007). Docking of ATP to Ca-ATPase: Considering protein domain motions. *J Chem Inf Model* 47 (3), 1171–1181, [10.1021/ci700067f](https://doi.org/10.1021/ci700067f)
157. Chugunov AO, Novoseletsky VN, Nolde DE, Arseniev AS, **Efremov RG** (2007). Method to assess packing quality of transmembrane α -helices in proteins. 2. Validation by "correct vs misleading" test. *J Chem Inf Model* 47 (3), 1163–1170, [10.1021/ci600517c](https://doi.org/10.1021/ci600517c)
158. Chugunov AO, Novoseletsky VN, Nolde DE, Arseniev AS, **Efremov RG** (2007). Method to assess packing quality of transmembrane α -helices in proteins. 1. Parametrization using structural data. *J Chem Inf Model* 47 (3), 1150–1162, [10.1021/ci600516x](https://doi.org/10.1021/ci600516x)
159. Polyansky AA, Volynsky PE, **Efremov RG** (2007). Computer simulations of membrane-lytic peptides: perspectives in drug design. *J Bioinform Comput Biol* 5 (2), 611–626, [10.1142/s0219720007002783](https://doi.org/10.1142/s0219720007002783)
160. Chugunov AO, Novoseletsky VN, Arseniev AS, **Efremov RG** (2007). A novel method for packing quality assessment of transmembrane α -helical domains in proteins. *Biochemistry (Mosc)* 72 (3), 293–300, [10.1134/S0006297907030066](https://doi.org/10.1134/S0006297907030066)
161. Pyrkov TV, Kosinsky YA, Arseniev AS, Priestle JP, Jacoby E, **Efremov RG** (2007). Complementarity of hydrophobic properties in ATP-protein binding: A new criterion to rank docking solutions. *Proteins* 66 (2), 388–398, [10.1002/prot.21122](https://doi.org/10.1002/prot.21122)
162. **Efremov RG**, Chugunov AO, Pyrkov TV, Priestle JP, Arseniev AS, Jacoby E (2007). Molecular lipophilicity in protein modeling and drug design. *Curr Med Chem* 14 (4), 393–415, [10.2174/092986707779941050](https://doi.org/10.2174/092986707779941050)
163. **Efremov RG**, Volynsky PE, Nolde DE, Vergoten G, Arseniev AS (2007). The membrane-proximal fusion domain of hiv-1 gp41 reveals sequence-specific and fine-tuning mechanism of membrane binding. *J Biomol Struct Dyn* 25 (2), 195–205, [10.1080/07391102.2007.10507169](https://doi.org/10.1080/07391102.2007.10507169)
164. Dubovskii PV, Volynsky PE, Polyansky AA, Chupin VV, **Efremov RG**, Arseniev AS (2006). Spatial structure and activity mechanism of a novel spider antimicrobial peptide. *Biochemistry* 45 (35), 10759–10767, [10.1021/bi060635w](https://doi.org/10.1021/bi060635w)
165. Volynsky PE, Bocharov EV, Nolde DE, Vereshaga YA, Mayzel ML, Mineev KS, Mineeva EA, Pustovalova YE, Gagnidze IA, **Efremov RG**, Arseniev AS (2006). Solution of the spatial structure of dimeric transmembrane domains of proteins by heteronuclear NMR spectroscopy and molecular modeling. *Biophysics (Oxf)* 51 (1), 23–27, [10.1134/S0006350906070050](https://doi.org/10.1134/S0006350906070050)
166. **Efremov RG**, Vereshaga YA, Volynsky PE, Nolde DE, Arseniev AS (2006). Association of transmembrane helices: What determines assembling of a dimer? *J Comput Aided Mol Des* 20 (1), 27–45, [10.1007/s10822-006-9034-6](https://doi.org/10.1007/s10822-006-9034-6)
167. Chugunov AO, Farce A, Chavatte P, **Efremov RG** (2006). Differences in binding sites of two melatonin receptors help to explain their selectivity to some melatonin analogs: A molecular modeling study. *J Biomol Struct Dyn* 24 (2), 91–107, [10.1080/07391102.2006.10507103](https://doi.org/10.1080/07391102.2006.10507103)
168. Vereshaga YA, Volynsky PE, Nolde DE, Arseniev AS, **Efremov RG** (2005). Helix interactions in membranes:

- Lessons from unrestrained Monte Carlo simulations. *J Chem Theory Comput* 1 (6), 1252–1264, [10.1021/ct0501250](https://doi.org/10.1021/ct0501250)
169. Volynsky PE, Polyansky AA, Simakov NA, Arseniev AS, **Efremov RG** (2005). Effect of lipid composition on the "membrane response" induced by a fusion peptide. *Biochemistry* 44 (44), 14626–14637, [10.1021/bi0514562](https://doi.org/10.1021/bi0514562)
 170. Polyansky AA, Volynsky PE, Nolde DE, Arseniev AS, **Efremov RG** (2005). Role of lipid charge in organization of water/lipid bilayer interface: Insights via computer simulations. *J Phys Chem B* 109 (31), 15052–15059, [10.1021/jp0510185](https://doi.org/10.1021/jp0510185)
 171. Dubovskii PV, Lesovoy DM, Dubinnyi MA, Konshina AG, Utkin YN, **Efremov RG**, Arseniev AS (2005). Interaction of three-finger toxins with phospholipid membranes: Comparison of S- and P-type cytotoxins. *Biochem J* 387 (3), 807–815, [10.1042/BJ20041814](https://doi.org/10.1042/BJ20041814)
 172. Polyansky AA, Kosinsky YA, **Efremov RG** (2004). Correlation of local changes in the temperature-dependent conformational flexibility of thioredoxins with their thermostability. *Russ. J. Bioorganic Chem.* 30 (5), 421–430, [10.1023/B:RUBI.0000043784.51859.41](https://doi.org/10.1023/B:RUBI.0000043784.51859.41)
 173. Morgan CT, Tsivkovskii R, Kosinsky YA, **Efremov RG**, Lutsenko S (2004). The distinct functional properties of the nucleotide-binding domain of ATP7B, the human copper-transporting ATPase: Analysis of the Wilson disease mutations E1064A, H1069Q, R1151H, and C1104F. *J Biol Chem* 279 (35), 36363–36371, [10.1074/jbc.M404553200](https://doi.org/10.1074/jbc.M404553200)
 174. **Efremov RG**, Kosinsky YA, Nolde DE, Tsivkovskii R, Arseniev AS, Lutsenko S (2004). Molecular modelling of the nucleotide-binding domain of Wilson's disease protein: Location of the ATP-binding site, domain dynamics and potential effects of the major disease mutations. *Biochem J* 382 (1), 293–305, [10.1042/BJ20040326](https://doi.org/10.1042/BJ20040326)
 175. Kosinsky YA, Volynsky PE, Lagant P, Vergoten G, Suzuki EI, Arseniev AS, **Efremov RG** (2004). Development of the force field parameters for phosphoimidazole and phosphohistidine. *J Comput Chem* 25 (11), 1313–1321, [10.1002/jcc.20055](https://doi.org/10.1002/jcc.20055)
 176. **Efremov RG**, Nolde DE, Konshina AG, Syrtcev NP, Arseniev AS (2004). Peptides and proteins in membranes: What can we learn via computer simulations? *Curr Med Chem* 11 (18), 2421–2442, [10.2174/0929867043364496](https://doi.org/10.2174/0929867043364496)
 177. Konshina AG, Volynsky PE, Arseniev AS, **Efremov RG** (2003). Interaction of cardiotoxin A5 with membrane: Role of conformational heterogeneity and hydrophobic properties. *Russ. J. Bioorganic Chem.* 29 (6), 523–533, [10.1023/B:RUBI.0000008892.75272.ab](https://doi.org/10.1023/B:RUBI.0000008892.75272.ab)
 178. Konshina AG, Volynskii PE, Arseniev AS, **Efremov RG** (2003). Interaction of cardiotoxin A5 with a membrane: role of conformational heterogeneity and hydrophilic properties. *Bioorg Khim* 29 (6), 577–588.
 179. Dioubankova NN, Malakhov AD, Stetsenko DA, Gait MJ, Volynsky PE, **Efremov RG**, Korshun VA (2003). Pyrenemethyl ara-uridine-2'-carbamate: A strong interstrand excimer in the major groove of a DNA duplex. *Chembiochem* 4 (9), 841–847, [10.1002/cbic.200300678](https://doi.org/10.1002/cbic.200300678)
 180. Tsivkovskii R, **Efremov RG**, Lutsenko S (2003). The role of the invariant His-1069 in folding and function of the Wilson's disease protein, the human copper-transporting ATPase ATP7B. *J Biol Chem* 278 (15), 13302–13308, [10.1074/jbc.M300034200](https://doi.org/10.1074/jbc.M300034200)
 181. Lutsenko S, **Efremov RG**, Tsivkovskii R, Walker JM (2002). Human copper-transporting ATPase ATP7B (The Wilson's Disease Protein): Biochemical properties and regulation. *J Bioenerg Biomembr* 34 (5), 351–362, [10.1023/A:1021297919034](https://doi.org/10.1023/A:1021297919034)
 182. **Efremov RG**, Volynsky PE, Nolde DE, Van Dalen A, De Kruijff B, Arseniev AS (2002). Monte Carlo simulations of voltage-driven translocation of a signal sequence. *FEBS Lett* 526 (13), 97–100, [10.1016/S0014-5793\(02\)03145-9](https://doi.org/10.1016/S0014-5793(02)03145-9)
 183. Abdullaev ZK, Bodrova ME, Chernyak BV, Dolgikh DA, Kluck RM, Pereverzev MO, Arseniev AS, **Efremov RG**, Kirpichnikov MP, Mokhova EN, Newmeyer DD, Roder H, Skulachev VP (2002). A cytochrome c mutant with high electron transfer and antioxidant activities but devoid of apoptogenic effect. *Biochem J* 362 (3), 749–754, [10.1042/0264-6021:3620749](https://doi.org/10.1042/0264-6021:3620749)
 184. **Efremov RG**, Volynsky PE, Nolde DE, Dubovskii PV, Arseniev AS (2002). Interaction of cardiotoxins with membranes: A molecular modeling study. *Biophys J* 83 (1), 144–153, [10.1016/S0006-3495\(02\)75156-4](https://doi.org/10.1016/S0006-3495(02)75156-4)
 185. Shenkarev ZO, Balashova TA, **Efremov RG**, Yakimenko ZA, Ovchinnikova TV, Raap J, Arseniev AS (2002). Spatial structure of zervamicin IIB bound to DPC micelles: Implications for voltage-gating. *Biophys J* 82 (2),

762–771, [10.1016/S0006-3495\(02\)75438-6](https://doi.org/10.1016/S0006-3495(02)75438-6)

186. **Efremov RG**, Volynsky PE, Dauchez MAM, Nolde DE, Arseniev AS, Alix AJP (2001). Assessment of conformation and energetics of the N-terminal part of elafin via computer simulations. *Theor Chem Acc* 106 (12), 55–61, [10.1007/s002140000237](https://doi.org/10.1007/s002140000237)
187. **Efremov R**, Volynsky P, Nolde D, Vergoten G, Arseniev A (2001). Implicit two-phase solvation model as a tool to assess conformation and energetics of proteins in membrane-mimetic media. *Theor Chem Acc* 106 (12), 48–54, [10.1007/s002140000220](https://doi.org/10.1007/s002140000220)
188. Nolde DE, Volynskii PE, Arseniev AS, **Efremov RG** (2000). Modeling of peptides and proteins in membrane environment. I. A solvation model mimicking a lipid bilayer. *Bioorg Khim* 26 (2), 140.
189. Volynskii PE, Nolde DE, Arseniev AS, **Efremov RG** (2000). Modeling of peptides and proteins in a membrane environment. II. Structural and energetic aspects of glycophorin A in a lipid bilayer. *Bioorg Khim* 26 (3), 171–172.
190. Volynskii PE, Nolde DE, Arseniev AS, **Efremov RG** (2000). Modeling of peptides and proteins in a membrane environment: II. Structural and energetic aspects of glycophorin A in a lipid bilayer. *Russ. J. Bioorganic Chem.* 26 (3), 143–151, [10.1007/BF02786338](https://doi.org/10.1007/BF02786338)
191. **Efremov RG**, Nolde DE, Volynsky PE, Chernyavsky AA, Dubovskii PV, Arseniev AS (1999). Factors important for fusogenic activity of peptides: Molecular modeling study of analogs of fusion peptide of influenza virus hemagglutinin. *FEBS Lett* 462 (12), 205–210, [10.1016/S0014-5793\(99\)01505-7](https://doi.org/10.1016/S0014-5793(99)01505-7)
192. Pashkov VS, Maslennikov IV, Tchikin LD, **Efremov RG**, Ivanov VT, Arseniev AS (1999). Spatial structure of the M2 transmembrane segment of the nicotinic acetylcholine receptor α -subunit. *FEBS Lett* 457 (1), 117–121, [10.1016/S0014-5793\(99\)01023-6](https://doi.org/10.1016/S0014-5793(99)01023-6)
193. **Efremov RG**, Nolde DE, Vergoten G, Arseniev AS (1999). A solvent model for simulations of peptides in bilayers. II. Membrane- spanning α -helices. *Biophys J* 76 (5), 2460–2471, [10.1016/S0006-3495\(99\)77401-1](https://doi.org/10.1016/S0006-3495(99)77401-1)
194. **Efremov RG**, Nolde DE, Vergoten G, Arseniev AS (1999). Peptides in membranes: Assessment of environmental effects via simulations using an implicit solvation model. *Theor Chem Acc* 101 (13), 170–174, [10.1007/s002140050425](https://doi.org/10.1007/s002140050425)
195. **Efremov RG**, Nolde DE, Vergoten G, Arseniev AS (1999). A solvent model for simulations of peptides in bilayers. I. Membrane- promoting α -helix formation. *Biophys J* 76 (5), 2448–2459, [10.1016/S0006-3495\(99\)77400-X](https://doi.org/10.1016/S0006-3495(99)77400-X)
196. **Efremov RG**, Vergoten G, Arseniev AS (1999). A new "hydrophobic template" method detects segments forming transmembrane α -helical bundles in ion channels. *Theor Chem Acc* 101 (13), 73–76, [10.1007/s002140050409](https://doi.org/10.1007/s002140050409)
197. Golovanov AP, **Efremov RG**, Jaravine VA, Vergoten G, Kirpichnikov MP, Arseniev AS (1998). A new method to characterize hydrophobic organization of proteins: Application to rational protein engineering of barnase. *J Biomol Struct Dyn* 15 (4), 673–687, [10.1080/07391102.1998.10508984](https://doi.org/10.1080/07391102.1998.10508984)
198. **Efremov RG**, Legret F, Vergoten G, Capron A, Bahr GM, Arseniev AS (1998). Molecular modeling of hiv-1 coreceptor ccr5 and exploring of conformational space of its extracellular domain in molecular dynamics simulation. *J Biomol Struct Dyn* 16 (1), 77–90, [10.1080/07391102.1998.10508229](https://doi.org/10.1080/07391102.1998.10508229)
199. **Efremov RG**, Vergoten G (1996). Recognition of transmembrane α -helical segments with environmental profiles. *Protein Eng* 9 (3), 253–263, [10.1093/protein/9.3.253](https://doi.org/10.1093/protein/9.3.253)
200. **Efremov RG**, Vergoten G (1996). Hydrophobic Organization of α -Helix Membrane Bundle in Bacteriorhodopsin. *Protein J* 15 (1), 63–76, [10.1007/BF01886812](https://doi.org/10.1007/BF01886812)
201. **Efremov RG**, Vergoten G (1995). Hydrophobic nature of membrane-spanning α -helical peptides as revealed by Monte Carlo simulations and molecular hydrophobicity potential analysis. *J Phys Chem* 99 (26), 10658–10666, [10.1021/j100026a033](https://doi.org/10.1021/j100026a033)
202. Golovanov AP, **Efremov RG**, Jaravine VA, Vergoten G, Arseniev AS (1995). Amino acid residue: is it structural or functional? *FEBS Lett* 375 (12), 162–166, [10.1016/0014-5793\(95\)01212-W](https://doi.org/10.1016/0014-5793(95)01212-W)
203. **Efremov RG**, Vergoten G (1995). The hydrophobic nature of membrane-spanning α -helices as revealed by Monte Carlo simulations and molecular hydrophobicity potential analysis. 99 (26), 10658–10666.
204. **Efremov RG**, Golovanov AP, Vergoten G, Alix AJ, Tsetlin VI, Arseniev AS (1995). Detailed assessment of spatial hydrophobic and electrostatic properties of 2d nmr-derived models of neurotoxin ii. *J Biomol Struct Dyn* 12 (5), 971–991, [10.1080/07391102.1995.10508791](https://doi.org/10.1080/07391102.1995.10508791)

205. **Efremov RG**, Gulyaev DI, Modyanov NN (1993). Application of three-dimensional molecular hydrophobicity potential to the analysis of spatial organization of membrane domains in proteins. III. Modeling of intramembrane moiety of Na⁺, K⁺-ATPase. *J Protein Chem* 12 (2), 143–152, [10.1007/BF01026035](https://doi.org/10.1007/BF01026035)
206. **Efremov RG**, Alix AJ, **Efremov RG** (1993). Environmental characteristics of residues in proteins: Three-dimensional molecular hydrophobicity potential approach. *J Biomol Struct Dyn* 11 (3), 483–507, [10.1080/07391102.1993.10508011](https://doi.org/10.1080/07391102.1993.10508011)
207. **Efremov RG**, Gulyaev DI, Modyanov NN (1992). Application of three-dimensional molecular hydrophobicity potential to the analysis of spatial organization of membrane protein domains. II. Optimization of hydrophobic contacts in transmembrane hairpin structures of Na⁺, K⁺-ATPase. *J Protein Chem* 11 (6), 699–708, [10.1007/BF01024971](https://doi.org/10.1007/BF01024971)
208. **Efremov RG**, Gulyaev DI, Vergoten G, Modyanov NN (1992). Application of three-dimensional molecular hydrophobicity potential to the analysis of spatial organization of membrane domains in proteins: I. Hydrophobic properties of transmembrane segments of Na⁺, K⁺-ATPase. *J Protein Chem* 11 (6), 665–675, [10.1007/BF01024968](https://doi.org/10.1007/BF01024968)
209. MODYANOV NN, VLADIMIROVA NM, GULYAEV DI, **EFREMOV RG** (1992). Architecture of the Sodium Pump Molecule: Vectorial Labeling and Computer Modeling. *Ann N Y Acad Sci* 671 (1), 134–146, [10.1111/j.1749-6632.1992.tb43791.x](https://doi.org/10.1111/j.1749-6632.1992.tb43791.x)
210. Modyanov N, Lutsenko S, Chertova E, **Efremov R**, Gulyaev D (1992). Transmembrane organization of the Na⁺,K⁺-ATPase molecule. *Acta Physiol Scand Suppl* 146 (607), 49–58.
211. Feofanov AV, Okolelov VI, Tatarinov AP, Martynova ES, **Efremov RG**, Nabiev IR, Pashchenko VZ, Manykin EA (1991). Selective analysis of nucleic acids in mycobacteria according to raman resonance spectroscopy data. *J APPL SPECTROSC* 55 (3), 877–883, [10.1007/BF00662414](https://doi.org/10.1007/BF00662414)
212. **Efremov RG**, Feofanov AV, Nabiev IR (1991). Computerized technique for the analysis of weak signals in UV Raman scattering from biological molecules. *J APPL SPECTROSC* 54 (5), 417–424, [10.1007/BF00660014](https://doi.org/10.1007/BF00660014)
213. Modyanov N, Lutsenko S, Chertova E, **Efremov R** (1991). Architecture of the sodium pump molecule: Probing the folding of the hydrophobic domain. *J Gen Physiol* 46 (44), 99–115.
214. **Efremov RG**, Feofanov AV, Dzhandzhugazyan KN, Modyanov NN, Nabiev IR (1990). Study of ATP binding in the active site of Na⁺,K⁺-ATPase as probed by ultraviolet resonance Raman spectroscopy. *FEBS Lett* 260 (2), 261–265, [10.1016/0014-5793\(90\)80117-2](https://doi.org/10.1016/0014-5793(90)80117-2)
215. **Efremov RG** (1990). Parallel Computing of Resonance Raman Intensities Using a Transputer Array. *DATA HANDL SCI TECHN* 6 (C), 21–30, [10.1016/S0922-3487\(08\)70153-9](https://doi.org/10.1016/S0922-3487(08)70153-9)
216. Nabiev IR, Dzhandzhugazyan KN, **Efremov RG**, Modyanov NN (1988). Binding of monovalent cations induces large changes in the secondary structure of Na⁺,K⁺-ATPase as probed by Raman spectroscopy. *FEBS Lett* 236 (1), 235–239, [10.1016/0014-5793\(88\)80321-1](https://doi.org/10.1016/0014-5793(88)80321-1)
217. Ovchinnikov YA, Arystarkhova EA, Arzamazova NM, Dzhandzhugazyan KN, **Efremov RG**, Nabiev IR, Modyanov NN (1988). Differentiated analysis of the secondary structure of hydrophilic and hydrophobic regions in α- and β-subunits of Na⁺,K⁺-ATPase by Raman spectroscopy. *FEBS Lett* 227 (2), 235–239, [10.1016/0014-5793\(88\)80905-0](https://doi.org/10.1016/0014-5793(88)80905-0)
218. Abdulaev NG, Nabiev IR, **Efremov RG**, Chumanov GD (1987). Retinal Schiff base position relative to the surfaces of photoreceptor disk. *FEBS Lett* 213 (1), 113–118, [10.1016/0014-5793\(87\)81474-6](https://doi.org/10.1016/0014-5793(87)81474-6)
219. Nabiev IR, **Efremov RG**, Chumanov GD (1985). The chromophore-binding site of bacteriorhodopsin. Resonance Raman and surface-enhanced resonance Raman spectroscopy and quantum chemical study. *J Biosci* 8 (12), 363–374, [10.1007/BF02703989](https://doi.org/10.1007/BF02703989)