Резюме: Чугунов Антон Олегович



Адрес

Федеральное государственное бюджетное учреждение науки Институт биоорганической химии им. академиков М.М. Шемякина и Ю.А. Овчинникова Российской академии наук, Москва, Россия

Контакты

batch2k@yandex.ru
+7(915)1088825
https://www.ibch.ru/ru/users/3

Образование

2008–2008	Брюссель, Бельгия	Стажировка в Свободном университете Брюсселя	Моделирование структуры комплекса вазоактивного интестинального пептида (ВИП) с его рецептором. Дизайн селективной пары неорецептор-неолиганд
2003–2006	Россия, Москва	Московский государственный университет им. М.В. Ломоносова, кафедра биоинженерии биологического факультета	Диплом кандидата физико-математических наук. Тема диссертации: «Новые подходы к молекулярному моделированию трансмембранных доменов рецепторов, действие которых опосредовано G-белками»
1998–2003	Россия, Москва	Московский государственный университет им. М.В. Ломоносова, кафедра биофизики биологического факультета	Диплом биофизика с отличием по теме: «Молекулярное моделирование человеческих рецепторов MT1 и MT2 мелатонина»
1994–1998	Россия, Зеленоград	ФМШ №1030	Окончил с золотой медалью

Работа в ИБХ

2018–наст.вр.	Старший научный сотрудник	
	Старший научный сотрудник	
2026–2026	Доцент	

Членство в советах и комиссиях ИБХ

	Ученый совет

Владение языками

Русский, Английский

Награды

2013	Медаль Европейской Академии	За работу «Компьютерное моделирование структуры и функций биомембран и мембранных белков»

Научные интересы

Меня интересуют принципы пространственной организации белков и механизмы их сворачивания. В первую очередь это касается мембранных белков и рецепторов, таких как G-белоксопряжённые рецепторы. Поскольку выбранная мной методическая сфера — это компьютерное моделирование структуры и динамики биомакромолекул, больше всего мне интересно, удастся ли когда-нибудь моделировать все эти важнейшие процессы на компьютере — без такой большой оглядки на эксперимент, которую всегда приходится делать теперь.

Степени и звания

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

Ссылки и контакты

http://biomolecula.ru, Scopus: 34569445900, Google Scholar, ORCID: 0000-0003-1331-3949, ResearcherID: D-1058-2009

Гранты и проекты

2027–наст.вр.	Омега-токи в мутантных потенциал-чувствительных доменах Nav1.4: от молекулярного моделирования к дизайну пептидных блокаторов

Публикации

1. Zaigraev MM, Zhivov EA, Chelyadinskii TR, Shulepko MA, Kulbatskii DS, Qing H, Zhenzhen Q, Kirpichnikov MP, Shenkarev ZO, **Chugunov AO**, Lyukmanova EN (2026). Mutagenesis-guided modeling of the Lynx1–α7 nicotinic acetylcholine receptor complex: An iterative feedback-driven approach. *Int J Biol Macromol* , 154624, 10.1016/j.ijbiomac.2026.154624
2. Popkova D, Menshov A, Sintsova O, Paramonov A, Kalina R, Panina I, Kalinovskii A, Osmakov D, Shamatova M, Dmitrenok P, **Chugunov A**, Kozlov S, Efremov R, Shenkarev Z, Gladkikh I, Leychenko E (2026). Novel β-defensin-like marine miniprotein magnificamide-2 with a remarkable potency in inhibiting mammalian α-amylases. *Int J Biol Macromol* 376, 153418, 10.1016/j.ijbiomac.2026.153418
3. Panina IS, Vlasova YS, Panina YS, Krasilnikov MS, Alferova VA, Korshun VA, **Chugunov AO** (2026). Towards molecular dynamics simulation of membrane-targeting photosensitizing antivirals. *Phys Chem Chem Phys* 28 (13), 8039–8046, 10.1039/d5cp04006j
4. Vorobeva AS, Kazakova EM, Garibova LA, Emekeeva DD, Kusainova TT, Fedorov II, Shelepchikov AA, Tretyakov AV, **Chugunov AO**, Gorshkov MV, Tarasova IA (2026). Proteasome Inhibition as a Cancer Type-Specific Off-Target Effect of Everolimus in Cancer Cells. *Biochemistry (Mosc)* 91 (2), 274–288, 10.1134/S0006297925603284
5. Shulepko MA, Che Y, Paramonov AS, Kocharovskaya MV, Kulbatskii DS, Ivanova AA, **Chugunov AO**, Bychkov ML, Kirichenko AV, Shenkarev ZO, Kirpichnikov MP, Lyukmanova EN (2025). Pro-Inflammatory Protein PSCA Is Upregulated in Neurological Diseases and Targets β2-Subunit-Containing nAChRs. *Biomolecules* 15 (10), , 10.3390/biom15101381
6. Trofimov YA, **Chugunov AO**, Vassilevski AA (2025). Secondary chelation through shared water provides ion selectivity in bacterial sodium channels. *Structure* 33 (8), 1446–1456.e3,

10.1016/j.str.2025.05.010
7. Scherbakov KA, Vassilevski AA, **Chugunov AO** (2025). Potassium channel selectivity is determined by square antiprismatic ion chelation. *Int J Biol Macromol* 305 (Pt 1), 140690, 10.1016/j.ijbiomac.2025.140690
8. Kvetkina AN, Oreshkov SD, Mironov PA, Zaigraev MM, Klimovich AA, Deriavko YV, Menshov AS, Kulbatskii DS, Logashina YA, Andreev YA, **Chugunov AO**, Kirpichnikov MP, Lyukmanova EN, Leychenko EV, Shenkarev ZO (2024). Sea Anemone Kunitz Peptide HCIQ2c1: Structure, Modulation of TRPA1 Channel, and Suppression of Nociceptive Reaction In Vivo. *Mar Drugs* 22 (12), 542, 10.3390/md22120542
9. Chernykh MA, Duzheva MA, Kuldyushev NA, Peigneur S, Berkut AA, Tytgat J, Vassilevski AA, **Chugunov AO** (2024). Scorpion Neurotoxin BeM9 Derivative Uncovers Unique Interaction Mode with Nav1.5 Sodium Channel Isoform. *Russ. J. Bioorganic Chem.* 50 (4), 1341–1350, 10.1134/S1068162024040083
10. Zavarzina II, Kuzmenkov AI, Dobrokhotov NA, Maleeva EE, Korolkova YV, Peigneur S, Tytgat J, Krylov NA, Vassilevski AA, **Chugunov AO** (2024). The scorpion toxin BeKm-1 blocks hERG cardiac potassium channels using an indispensable arginine residue. *FEBS Lett* 598 (8), 889–901, 10.1002/1873-3468.14850
11. Karnaukhov VK, Shcherbinin DS, **Chugunov AO**, Chudakov DM, Efremov RG, Zvyagin IV, Shugay M (2024). Structure-based prediction of T cell receptor recognition of unseen epitopes using TCRen*NAT COMPUT SCI* 4 (7), 510–521, 10.1038/s43588-024-00653-0
12. Lyukmanova EN, Zaigraev MM, Kulbatskii DS, Isaev AB, Kukushkin ID, Bychkov ML, Shulepko MA, **Chugunov AO**, Kirpichnikov MP (2023). Molecular Basis for Mambalgin-2 Interaction with Heterotrimeric α-ENaC/ASIC1a/γ-ENaC Channels in Cancer Cells. *Toxins (Basel)* 15 (10), 612, 10.3390/toxins15100612
13. **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), 12369, 10.3390/ijms241512369
14. 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
15. Zaigraev MM, Lyukmanova EN, Paramonov AS, Shenkarev ZO, **Chugunov AO** (2022). Orientational Preferences of GPI-Anchored Ly6/uPAR Proteins. *Int J Mol Sci* 24 (1), 11, 10.3390/ijms24010011
16. Shenkarev ZO, Chesnokov YM, Zaigraev MM, **Chugunov AO**, Kulbatskii DS, Kocharovskaya MV, Paramonov AS, Bychkov ML, Shulepko MA, Nolde DE, Kamyshinsky RA, Yablokov EO, Ivanov AS, Kirpichnikov MP, Lyukmanova EN (2022). Membrane-mediated interaction of non-conventional snake three-finger toxins with nicotinic acetylcholine receptors. *Commun Biol* 5 (1), 1344, 10.1038/s42003-022-04308-6
17. 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
18. 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
19. **Chugunov AO**, Potapova NA, Klimenko NS, Tatarskiy VV, Georgieva SG, Soshnikova NV (2021). Conserved structure and evolution of dpf domain of phf10—the specific subunit of pbaf chromatin remodeling complex. *Int J Mol Sci* 22 (20), , 10.3390/ijms222011134
20. 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
21. 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
22. 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
23. 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
24. Shulepko MA, Bychkov ML, Shenkarev ZO, Kulbatskii DS, Makhonin AM, Paramonov AS, **Chugunov AO**, Kirpichnikov MP, Lyukmanova EN (2021). Biochemical basis of skin disease Mal de Meleda: SLURP-1 mutants differently affect keratinocyte proliferation and apoptosis. *J Invest Dermatol* 141 (9), 2229–2237, 10.1016/j.jid.2021.01.035
25. Belozerova 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
26. 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
27. 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
28. 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
29. 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
30. 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
31. Myshkin MY, Männikkö R, Krumkacheva OA, Kulbatskii DS, **Chugunov AO**, Berkut AA, Paramonov AS, Shulepko MA, Fedin MV, Hanna MG, Kullmann DM, Bagryanskaya EG, Arseniev AS, Kirpichnikov MP, Lyukmanova EN, Vassilevski AA, Shenkarev ZO (2019). Cell-Free Expression of Sodium Channel Domains for Pharmacology Studies. Noncanonical Spider Toxin Binding Site in the Second Voltage-Sensing Domain of Human Nav1.4 Channel. *Front Pharmacol* 10, 953, 10.3389/fphar.2019.00953
32. 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
33. 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
34. 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
35. 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
36. Paramonov AS, Lyukmanova EN, Myshkin MY, Shulepko MA, Kulbatskii DS, Petrosian NS, **Chugunov AO**, Dolgikh DA, Kirpichnikov MP, Arseniev AS, Shenkarev ZO (2017). NMR investigation of the isolated second voltage-sensing domain of human Nav1.4 channel. *BIOCHIM BIOPHYS ACTA* 1859 (3), 1–33, 10.1016/j.bbamem.2017.01.004
37. 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
38. **(конференция)** Панина ИС, Нольде ДЕ, **Чугунов АО**, Ефремов РГ (2016). Структурно-динамическая модель комплекса лантибиотика низин с липидом-II в биомембране. 1, 263–267.
39. **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
40. 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
41. 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
42. Kuzmenkov AI, Krylov NA, **Chugunov AO**, Grishin EV, Vassilevski AA (2016). Kalium: A database of potassium channel toxins from scorpion venom. *Database (Oxford)* 2016, baw056, 10.1093/database/baw056
43. 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
44. 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
45. **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
46. **Чугунов АО**, Ефремов РГ (2014). Поверхность молекулы -- источник биологической информации. (10), 3–10.
47. Lyukmanova EN, Shulepko MA, Bychkov ML, Shenkarev ZO, Paramonov AS, **Chugunov AO**, Arseniev AS, Dolgikh DA, Kirpichnikov MP (2014). Human SLURP-1 and SLURP-2 Proteins Acting on Nicotinic Acetylcholine Receptors Reduce Proliferation of Human Colorectal Adenocarcinoma HT-29 Cells. *Acta Naturae* 6 (4), 60–6.
48. 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

49. Lyukmanova EN, Shulepko MA, Bychkov ML, Shenkarev ZO, Paramonov AS, **Chugunov AO**, Arseniev AS, Dolgikh DA, Kirpichnikov MP (2014). Human SLURP-1 and SLURP-2 proteins Acting on nicotinic acetylcholine receptors reduce proliferation of human colorectal adenocarcinoma HT-29 cells. *Acta Naturae* 6 (23), 60–66, 10.32607/20758251-2014-6-4-60-66
50. 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
51. **Чугунов АО**, Василевский АА (2013). Эволюционная «гонка вооружений»: нейротоксины против ионных каналов. 11, 42–48.
52. **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
53. **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
54. **Чугунов АО**, Нольде ДЕ, Пыркова ДВ, Полянский АА, Пентковский ВМ, Ефремов РГ (2013). На пути к новым антибиотикам. 12, 34–36.
55. **Чугунов АО**, Полянский АА, Ефремов РГ (2013). Физическая водобоязнь. 1, 24–34.
56. 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
57. 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
58. Semenova AA, **Chugunov AO**, Dubovskii PV, Chupin VV, Volynsky PE, Boldyrev IA (2012). The role of chain rigidity in lipid self-association: Comparative study of dihexanoyl- and disorbyl-phosphatidylcholines. *Chem Phys Lipids* 165 (4), 382–386, 10.1016/j.chemphyslip.2011.12.004
59. **Чугунов АО**, Полянский АА, Ефремов РГ (2012). Липидный фундамент жизни. (3), 3–12.
60. **(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, 10.2174/978160805464011306001 3
61. Deyev IE, Sohet F, Vassilenko KP, Serova OV, Popova NV, Zozulya SA, Burova EB, Houillier P, Rzhevsky DI, Berchatova AA, Murashev AN, **Chugunov AO**, Efremov RG, NikolSky 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
62. **Чугунов АО**, Ефремов РГ (2010). Компьютерные игры в молекулярную биофизику. (12), 36–43.
63. **Chugunov AO**, Simms J, Poyner DR, Dehouck Y, Rooman M, Gilis D, Langer I (2010). Evidence that interaction between conserved residues in transmembrane helices 2, 3, and 7 are crucial for human VPAC1 receptor activation. *Mol Pharmacol* 78 (3), 394–401, 10.1124/mol.110.063578
64. 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
65. **Chugunov AO**, Efremov RG (2009). Prediction of the spatial structure of proteins: emphasis on membrane targets. *Bioorg Khim* 35 (6), 744–760.
66. **Чугунов АО**, Ефремов РГ (2009). Предсказание пространственной структуры белков: акцент на мембранных мишенях. 35 (6), 1–17.
67. **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
68. 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

69. 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 MT1and MT2receptors. *Eur J Med Chem* 43 (9), 1926–1944, 10.1016/j.ejmech.2007.12.001
70. **Chugunov AO**, Novoseletsky VN, Nolde DE, Arseniev AS, Efremov RG (2007). Method to assess packing quality of transmembrane a-helices in proteins. 1. Parametrization using structural data. *J Chem Inf Model* 47 (3), 1150–1162, 10.1021/ci600516x
71. **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
72. **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
73. 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
74. **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