

Roman G Efremov

List of Publications by Year in descending order

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197
papers

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citations

94381

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155592

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205
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205
docs citations

205
times ranked

4198
citing authors

#	ARTICLE	IF	CITATIONS
1	Small Amphiphilic Peptides: Activity Against a Broad Range of Drug-Resistant Bacteria and Structural Insight into Membranolytic Properties. <i>Journal of Medicinal Chemistry</i> , 2022, 65, 665-687.	2.9	8
2	Differences in Medium-Induced Conformational Plasticity Presumably Underlie Different Cytotoxic Activity of Ricin and Viscumin. <i>Biomolecules</i> , 2022, 12, 295.	1.8	1
3	Variability in the Spatial Structure of the Central Loop in Cobra Cytotoxins Revealed by X-ray Analysis and Molecular Modeling. <i>Toxins</i> , 2022, 14, 149.	1.5	6
4	Molecular Dynamics of DHHC20 Acyltransferase Suggests Principles of Lipid and Protein Substrate Selectivity. <i>International Journal of Molecular Sciences</i> , 2022, 23, 5091.	1.8	6
5	Artificial Peptide Ligand of Potassium Channel KV1.1 with High Selectivity. <i>Journal of Evolutionary Biochemistry and Physiology</i> , 2021, 57, 386-403.	0.2	4
6	libxtc: an efficient library for reading XTC-compressed MD trajectory data. <i>BMC Research Notes</i> , 2021, 14, 124.	0.6	9
7	Dynamic "Molecular Portraits" of Biomembranes Drawn by Their Lateral Nanoscale Inhomogeneities. <i>International Journal of Molecular Sciences</i> , 2021, 22, 6250.	1.8	5
8	Potassium channel blocker crafted by Î±-hairpinin scaffold engineering. <i>Biophysical Journal</i> , 2021, 120, 2471-2481.	0.2	3
9	Derivative of Scorpion Neurotoxin BeM9 Is Selective for Insect Voltage-Gated Sodium Channels. <i>Russian Journal of Bioorganic Chemistry</i> , 2021, 47, 854-863.	0.3	0
10	Structural mechanism of heat-induced opening of a temperature-sensitive TRP channel. <i>Nature Structural and Molecular Biology</i> , 2021, 28, 564-572.	3.6	76
11	Molecular Dynamics Insight into the Lipid II Recognition by Type A Lantibiotics: Nisin, Epidermin, and Gallidermin. <i>Micromachines</i> , 2021, 12, 1169.	1.4	9
12	Human Three-Finger Protein Lypd6 Is a Negative Modulator of the Cholinergic System in the Brain. <i>Frontiers in Cell and Developmental Biology</i> , 2021, 9, 662227.	1.8	10
13	Stepwise Insertion of Cobra Cardiotoxin CT2 into a Lipid Bilayer Occurs as an Interplay of Protein and Membrane "Dynamic Molecular Portraits". <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 385-399.	2.5	6
14	All-d-Enantiomeric Peptide D3 Designed for Alzheimer's Disease Treatment Dynamically Interacts with Membrane-Bound Amyloid-Î² Precursors. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 16464-16479.	2.9	7
15	Antibacterial activity of cardiotoxin-like basic polypeptide from cobra venom. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2020, 30, 126890.	1.0	4
16	Sevanol and Its Analogues: Chemical Synthesis, Biological Effects and Molecular Docking. <i>Pharmaceuticals</i> , 2020, 13, 163.	1.7	2
17	Dimeric states of transmembrane domains of insulin and IGF-1R receptors: Structures and possible role in activation. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2020, 1862, 183417.	1.4	6
18	Tuning of Molecular Electrostatic Potential Enables Efficient Charge Transport in Crystalline Azaacenes: A Computational Study. <i>International Journal of Molecular Sciences</i> , 2020, 21, 5654.	1.8	6

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19	Structure of Supramers Formed by the Amphiphile Biotinâ€CMGâ€DOPE. <i>ChemistryOpen</i> , 2020, 9, 641-648.	0.9	5
20	Environmental and dynamic effects explain how nisin captures membrane-bound lipid II. <i>Scientific Reports</i> , 2020, 10, 8821.	1.6	21
21	Tuning Scorpion Toxin Selectivity: Switching From KV1.1 to KV1.3. <i>Frontiers in Pharmacology</i> , 2020, 11, 1010.	1.6	8
22	Impact of external amino acids on fluorescent protein chromophore biosynthesis revealed by molecular dynamics and mutagenesis studies. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2020, 206, 111853.	1.7	5
23	Complex approach for analysis of snake venom Î±-neurotoxins binding to HAP, the high-affinity peptide. <i>Scientific Reports</i> , 2020, 10, 3861.	1.6	11
24	The Role of Protein-Lipid Interactions in the Functioning of Bitopic Membrane Proteins. <i>Biophysical Journal</i> , 2020, 118, 211a.	0.2	0
25	Transmembrane Peptides as Inhibitors of Protein-Protein Interactions: An Efficient Strategy to Target Cancer Cells?. <i>Frontiers in Oncology</i> , 2020, 10, 519.	1.3	21
26	Probing temperature and capsaicin-induced activation of TRPV1 channel via computationally guided point mutations in its pore and TRP domains. <i>International Journal of Biological Macromolecules</i> , 2020, 158, 1175-1183.	3.6	3
27	Transmembrane Peptides as a New Strategy to Inhibit Neuraminidase-1 Activation. <i>Frontiers in Cell and Developmental Biology</i> , 2020, 8, 611121.	1.8	11
28	Confined Dynamics of Water in Transmembrane Pore of TRPV1 Ion Channel. <i>International Journal of Molecular Sciences</i> , 2019, 20, 4285.	1.8	4
29	Protein surface topography as a tool to enhance the selective activity of a potassium channel blocker. <i>Journal of Biological Chemistry</i> , 2019, 294, 18349-18359.	1.6	10
30	Specific refolding pathway of viscumin A chain in membrane-like medium reveals a possible mechanism of toxin entry into cell. <i>Scientific Reports</i> , 2019, 9, 413.	1.6	3
31	Elastic fibers and elastin receptor complex: Neuraminidase-1 takes the center stage. <i>Matrix Biology</i> , 2019, 84, 57-67.	1.5	27
32	Kalium 2.0, a comprehensive database of polypeptide ligands of potassium channels. <i>Scientific Data</i> , 2019, 6, 73.	2.4	28
33	Dielectric-Dependent Strength of Interlipid Hydrogen Bonding in Biomembranes: Model Case Study. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2765-2775.	2.5	8
34	Familial L723P Mutation Can Shift the Distribution between the Alternative APP Transmembrane Domain Cleavage Cascades by Local Unfolding of the Î±-Cleavage Site Suggesting a Straightforward Mechanism of Alzheimerâ€™s Disease Pathogenesis. <i>ACS Chemical Biology</i> , 2019, 14, 1573-1582.	1.6	13
35	Dynamic â€œMolecular Portraitsâ€ of Proteins and Cell Membranes: A Computational View. <i>Biophysical Journal</i> , 2019, 116, 205a.	0.2	0
36	Atomistic mechanism of the constitutive activation of PDGFRA via its transmembrane domain. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2019, 1863, 82-95.	1.1	8

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37	Proton-independent activation of acid-sensing ion channel 3 by an alkaloid, lindoldhamine, from <i>Laurus nobilis</i> . <i>British Journal of Pharmacology</i> , 2018, 175, 924-937.	2.7	14
38	Structural basis of the signal transduction via transmembrane domain of the human growth hormone receptor. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2018, 1862, 1410-1420.	1.1	28
39	Impact of membrane partitioning on the spatial structure of an S-type cobra cytotoxin. <i>Journal of Biomolecular Structure and Dynamics</i> , 2018, 36, 3463-3478.	2.0	13
40	Fine Tuning of Microscopic Properties in Two-Component Zwitterionic-Anionic Lipid Bilayers: Determinant Role of H-Bonding. <i>Biophysical Journal</i> , 2018, 114, 601a.	0.2	2
41	Behavior of Doxorubicin Lipophilic Conjugates in Liposomal Lipid Bilayers. <i>Russian Journal of Bioorganic Chemistry</i> , 2018, 44, 732-739.	0.3	0
42	Lipid II as a Target for Novel Antibiotics: Structural and Molecular Dynamics Studies. <i>Russian Journal of Bioorganic Chemistry</i> , 2018, 44, 653-664.	0.3	1
43	Crystal Structure of the pH-Dependent Green Fluorescent Protein WasCFP with a Tryptophan-Based Chromophore at an Extremely Low pH of 2.0. <i>Russian Journal of Bioorganic Chemistry</i> , 2018, 44, 640-644.	0.3	0
44	Probing the effect of membrane contents on transmembrane protein-protein interaction using solution NMR and computer simulations. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2018, 1860, 2486-2498.	1.4	10
45	KV1.2 channel-specific blocker from <i>Mesobuthus eupeus</i> scorpion venom: Structural basis of selectivity. <i>Neuropharmacology</i> , 2018, 143, 228-238.	2.0	20
46	The role of hydrophobic /hydrophilic balance in the activity of structurally flexible vs. rigid cytolytic polypeptides and analogs developed on their basis. <i>Expert Review of Proteomics</i> , 2018, 15, 873-886.	1.3	8
47	Improving therapeutic potential of antibacterial spider venom peptides: coarse-grain molecular dynamics guided approach. <i>Future Medicinal Chemistry</i> , 2018, 10, 2309-2322.	1.1	7
48	C-Terminal residues in small potassium channel blockers OdK1 and OSK3 from scorpion venom fine-tune the selectivity. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2017, 1865, 465-472.	1.1	8
49	Temperature-Sensitive Gating of TRPV1 Channel as Probed by Atomistic Simulations. <i>Biophysical Journal</i> , 2017, 112, 506a.	0.2	0
50	The Conformation of the Epidermal Growth Factor Receptor Transmembrane Domain Dimer Dynamically Adapts to the Local Membrane Environment. <i>Biochemistry</i> , 2017, 56, 1697-1705.	1.2	39
51	Cardiotoxins: Functional Role of Local Conformational Changes. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 2799-2810.	2.5	15
52	Structural and Dynamic "Portraits" of Recombinant and Native Cytotoxin I from <i>Naja oxiana</i> : How Close Are They?. <i>Biochemistry</i> , 2017, 56, 4468-4477.	1.2	8
53	Molecular modeling of biomembranes and their complexes with protein transmembrane α -helices. <i>AIP Conference Proceedings</i> , 2017, , .	0.3	0
54	Why human anti-Gal β 1 \rightarrow 4Gal β 1 \rightarrow 4Glc natural antibodies do not recognize the trisaccharide on erythrocyte membrane? Molecular dynamics and immunochemical investigation. <i>Molecular Immunology</i> , 2017, 90, 87-97.	1.0	8

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55	Helix-helix interactions in membrane domains of bitopic proteins: Specificity and role of lipid environment. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2017, 1859, 561-576.	1.4	72
56	Three-dimensional structure of a pH-dependent fluorescent protein WasCFP with a tryptophan based deprotonated chromophore. <i>Russian Journal of Bioorganic Chemistry</i> , 2016, 42, 612-618.	0.3	1
57	New Insights into Molecular Organization of Human Neuraminidase-1: Transmembrane Topology and Dimerization Ability. <i>Scientific Reports</i> , 2016, 6, 38363.	1.6	44
58	Stochastic but Fine-Tuned: Dualism in Cell Membranes' Organization as Revealed by Computer Simulations. <i>Biophysical Journal</i> , 2016, 110, 567a.	0.2	0
59	High-Affinity $\hat{\pm}$ -Conotoxin PnIA Analogs Designed on the Basis of the Protein Surface Topography Method. <i>Scientific Reports</i> , 2016, 6, 36848.	1.6	23
60	Secreted Isoform of Human Lynx1 (SLURP-2): Spatial Structure and Pharmacology of Interactions with Different Types of Acetylcholine Receptors. <i>Scientific Reports</i> , 2016, 6, 30698.	1.6	34
61	Temperature-sensitive gating of TRPV1 channel as probed by atomistic simulations of its trans- and juxtamembrane domains. <i>Scientific Reports</i> , 2016, 6, 33112.	1.6	49
62	Central loop of non-conventional toxin WTX from <i>Naja kaouthia</i> is important for interaction with nicotinic acetylcholine receptors. <i>Toxicon</i> , 2016, 119, 274-279.	0.8	18
63	Dynamic Structural/Amphiphilic $\hat{\pm}$ Portrait of Biomembranes as their Fundamental Property Relevant to Function: Results of Atomistic Simulations. <i>Biophysical Journal</i> , 2015, 108, 78a.	0.2	1
64	Cobra cytotoxins: determinants of antibacterial activity. <i>Mendeleev Communications</i> , 2015, 25, 70-71.	0.6	6
65	Rational design of new ligands for nicotinic receptors on the basis of $\hat{\pm}$ -conotoxin PnIA. <i>Doklady Biochemistry and Biophysics</i> , 2015, 461, 106-109.	0.3	3
66	Structural Insight into Specificity of Interactions between Nonconventional Three-finger Weak Toxin from <i>Naja kaouthia</i> (WTX) and Muscarinic Acetylcholine Receptors. <i>Journal of Biological Chemistry</i> , 2015, 290, 23616-23630.	1.6	37
67	Latacins: versatile spider venom peptides. <i>Cellular and Molecular Life Sciences</i> , 2015, 72, 4501-4522.	2.4	54
68	Adaptable Lipid Matrix Promotes Protein-Protein Association in Membranes. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4415-4426.	2.3	21
69	Role of the Lipid Environment in the Dimerization of Transmembrane Domains of Glycophorin A. <i>Acta Naturae</i> , 2015, 7, 122-127.	1.7	7
70	Role of the Lipid Environment in the Dimerization of Transmembrane Domains of Glycophorin A. <i>Acta Naturae</i> , 2015, 7, 122-7.	1.7	3
71	Interaction of linear cationic peptides with phospholipid membranes and polymers of sialic acid. <i>Biochemistry (Moscow)</i> , 2014, 79, 459-468.	0.7	7
72	PREDDIMER: a web server for prediction of transmembrane helical dimers. <i>Bioinformatics</i> , 2014, 30, 889-890.	1.8	77

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73	End-group differentiating ozonolysis of furocoumarins. RSC Advances, 2014, 4, 61277-61280.	1.7	3
74	Deciphering Fine Molecular Details of Proteinsâ€™ Structure and Function with a Protein Surface Topography (PST) Method. Journal of Chemical Information and Modeling, 2014, 54, 1189-1199.	2.5	28
75	Liquid but Durable: Molecular Dynamics Simulations Explain the Unique Properties of Archaeal-Like Membranes. Scientific Reports, 2014, 4, 7462.	1.6	42
76	Lipid-II forms potential "landing terrain" for lantibiotics in simulated bacterial membrane. Scientific Reports, 2013, 3, 1678.	1.6	56
77	Modular Organization of Î±-Toxins from Scorpion Venom Mirrors Domain Structure of Their Targets, Sodium Channels. Journal of Biological Chemistry, 2013, 288, 19014-19027.	1.6	31
78	Nontrivial Behavior of Water in the Vicinity and Inside Lipid Bilayers As Probed by Molecular Dynamics Simulations. ACS Nano, 2013, 7, 9428-9442.	7.3	34
79	Interaction between the Elastin Peptide VGVAPG and Human Elastin Binding Protein. Journal of Biological Chemistry, 2013, 288, 1317-1328.	1.6	50
80	Dynamic clustering of lipids in hydrated two-component membranes: results of computer modeling and putative biological impact. Journal of Biomolecular Structure and Dynamics, 2013, 31, 87-95.	2.0	12
81	Role of Dimerization Efficiency of Transmembrane Domains in Activation of Fibroblast Growth Factor Receptor 3. Journal of the American Chemical Society, 2013, 135, 8105-8108.	6.6	20
82	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. Journal of Bacteriology, 2013, 195, 95-104.	1.0	9
83	Cobra Cardiotoxins: Membrane Interactions and Pharmacological Potential. Current Medicinal Chemistry, 2013, 21, 270-287.	1.2	48
84	Recent Advances in Computational Modeling of Î±-Helical Membrane-Active Peptides. Current Protein and Peptide Science, 2012, 13, 644-657.	0.7	19
85	Structure and Dynamics of Cardiotoxins. Current Protein and Peptide Science, 2012, 13, 570-584.	0.7	58
86	Dissecting structural basis of the unique substrate selectivity of human enteropeptidase catalytic subunit. Journal of Biomolecular Structure and Dynamics, 2012, 30, 62-73.	2.0	3
87	Structure-Functional Insight into Transmembrane Helix Dimerization by Protein Engineering, Molecular Modeling and Heteronuclear NMR Spectroscopy. Biophysical Journal, 2012, 102, 470a.	0.2	1
88	Multistate Organization of Transmembrane Helical Protein Dimers Governed by the Host Membrane. Journal of the American Chemical Society, 2012, 134, 14390-14400.	6.6	63
89	How broadly tuned olfactory receptors equally recognize their agonists. Human OR1G1 as a test case. Cellular and Molecular Life Sciences, 2012, 69, 4205-4213.	2.4	64
90	Recognition Specificity of Proteins and Biomembranes: A Computational View. Biophysical Journal, 2012, 102, 434a.	0.2	0

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91	System-Specific Scoring Functions: Application to Guanine-Containing Ligands and Thrombin. NATO Science for Peace and Security Series B: Physics and Biophysics, 2012, , 21-37.	0.2	0
92	Molecular Lipophilicity in Protein Modeling and Drug Design. , 2012, , 249-290.		0
93	Structural Aspects of Transmembrane Domain Interactions of Receptor Tyrosine Kinases. Biophysical Journal, 2011, 100, 207a.	0.2	1
94	Insulin Receptor-Related Receptor as an Extracellular Alkali Sensor. Cell Metabolism, 2011, 13, 679-689.	7.2	92
95	Linker and/or transmembrane regions of influenza A/Group-1, A/Group-2, and type B virus hemagglutinins are packed differently within trimers. Biochimica Et Biophysica Acta - Biomembranes, 2011, 1808, 1843-1854.	1.4	38
96	Snake Cytotoxins Bind to Membranes via Interactions with Phosphatidylserine Head Groups of Lipids. PLoS ONE, 2011, 6, e19064.	1.1	53
97	Atomic-scale lateral heterogeneity and dynamics of two-component lipid bilayers composed of saturated and unsaturated phosphatidylcholines. Soft Matter, 2011, 7, 2569.	1.2	27
98	Lateral clustering of lipids in hydrated bilayers composed of dioleoylphosphatidylcholine and dipalmitoylphosphatidylcholine. Biochemistry (Moscow) Supplement Series A: Membrane and Cell Biology, 2011, 5, 278-285.	0.3	2
99	Structural, dynamic, and functional aspects of helix association in membranes. Advances in Protein Chemistry and Structural Biology, 2011, 83, 129-161.	1.0	12
100	Dimeric Structure of the Transmembrane Domain of Glycophorin A in Lipidic and Detergent Environments. Acta Naturae, 2011, 3, 90-98.	1.7	37
101	Dimeric structure of the transmembrane domain of glycophorin a in lipidic and detergent environments. Acta Naturae, 2011, 3, 90-8.	1.7	23
102	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 Crystallographica Section D: Biological Crystallography, 2010, 66, 51-60.	2.5	18
103	Analysis of hydrophobic interactions of antagonists with the beta2-adrenergic receptor. SAR and QSAR in Environmental Research, 2010, 21, 37-55.	1.0	8
104	Structure elucidation of dimeric transmembrane domains of bitopic proteins. Cell Adhesion and Migration, 2010, 4, 284-298.	1.1	34
105	Left-Handed Dimer of EphA2 Transmembrane Domain: Helix Packing Diversity among Receptor Tyrosine Kinases. Biophysical Journal, 2010, 98, 881-889.	0.2	100
106	Antimicrobial Peptides Induce Growth of Phosphatidylglycerol Domains in a Model Bacterial Membrane. Journal of Physical Chemistry Letters, 2010, 1, 3108-3111.	2.1	65
107	Computer simulations and modeling-assisted ToxR screening in deciphering 3D structures of transmembrane α -helical dimers: ephrin receptor A1. Physical Biology, 2010, 7, 016014.	0.8	11
108	Anionic Lipids: Determinants of Binding Cytotoxins from Snake Venom on the Surface of Cell Membranes. Acta Naturae, 2010, 2, 88-95.	1.7	9

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109	Anionic lipids: determinants of binding cytotoxins from snake venom on the surface of cell membranes. <i>Acta Naturae</i> , 2010, 2, 88-96.	1.7	5
110	PLATINUM: a web tool for analysis of hydrophobic/hydrophilic organization of biomolecular complexes. <i>Bioinformatics</i> , 2009, 25, 1201-1202.	1.8	159
111	N-terminal amphipathic helix as a trigger of hemolytic activity in antimicrobial peptides: A case study in laticins. <i>FEBS Letters</i> , 2009, 583, 2425-2428.	1.3	34
112	Adaptation of a Membrane-active Peptide to Heterogeneous Environment. II. The Role of Mosaic Nature of the Membrane Surface. <i>Journal of Physical Chemistry B</i> , 2009, 113, 1120-1126.	1.2	23
113	Specific Membrane Binding of Neurotoxin II Can Facilitate Its Delivery to Acetylcholine Receptor. <i>Biophysical Journal</i> , 2009, 97, 2089-2097.	0.2	31
114	Adaptation of a Membrane-active Peptide to Heterogeneous Environment. I. Structural Plasticity of the Peptide. <i>Journal of Physical Chemistry B</i> , 2009, 113, 1107-1119.	1.2	36
115	The Role of Stacking Interactions in Complexes of Proteins with Adenine and Guanine Fragments of Ligands. <i>Acta Naturae</i> , 2009, 1, 124-127.	1.7	17
116	Complementarity of Hydrophobic/Hydrophilic Properties In Protein-Ligand Complexes: A New Tool to Improve Docking Results. <i>NATO Science for Peace and Security Series B: Physics and Biophysics</i> , 2009, , 21-41.	0.2	1
117	The role of stacking interactions in complexes of proteins with adenine and Guanine fragments of ligands. <i>Acta Naturae</i> , 2009, 1, 124-7.	1.7	6
118	Homology modeling of MT1 and MT2 receptors. <i>European Journal of Medicinal Chemistry</i> , 2008, 43, 1926-1944.	2.6	23
119	Spatial Structure and pH-dependent Conformational Diversity of Dimeric Transmembrane Domain of the Receptor Tyrosine Kinase EphA1. <i>Journal of Biological Chemistry</i> , 2008, 283, 29385-29395.	1.6	100
120	Spatial Structure of the Dimeric Transmembrane Domain of the Growth Factor Receptor ErbB2 Presumably Corresponding to the Receptor Active State. <i>Journal of Biological Chemistry</i> , 2008, 283, 6950-6956.	1.6	189
121	Ligand-specific scoring functions: improved ranking of docking solutions. <i>SAR and QSAR in Environmental Research</i> , 2008, 19, 91-99.	1.0	11
122	Three-Dimensional Structure/Hydrophobicity of Laticins Specifies Their Mode of Membrane Activity. <i>Biochemistry</i> , 2008, 47, 3525-3533.	1.2	38
123	COMPUTER SIMULATIONS OF MEMBRANE-LYTIC PEPTIDES: PERSPECTIVES IN DRUG DESIGN. <i>Journal of Bioinformatics and Computational Biology</i> , 2007, 05, 611-626.	0.3	9
124	Unique Dimeric Structure of BNip3 Transmembrane Domain Suggests Membrane Permeabilization as a Cell Death Trigger. <i>Journal of Biological Chemistry</i> , 2007, 282, 16256-16266.	1.6	121
125	The Membrane-proximal Fusion Domain of HIV-1 GP41 Reveals Sequence-specific and Fine-tuning Mechanism of Membrane Binding. <i>Journal of Biomolecular Structure and Dynamics</i> , 2007, 25, 195-205.	2.0	2
126	Docking of ATP to Ca-ATPase: Considering Protein Domain Motions. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 1171-1181.	2.5	11

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127	Method To Assess Packing Quality of Transmembrane α -Helices in Proteins. 1. Parametrization Using Structural Data. Journal of Chemical Information and Modeling, 2007, 47, 1150-1162.	2.5	7
128	Molecular Lipophilicity in Protein Modeling and Drug Design. Current Medicinal Chemistry, 2007, 14, 393-415.	1.2	128
129	Method To Assess Packing Quality of Transmembrane α -Helices in Proteins. 2. Validation by "Correct vs Misleading" Test. Journal of Chemical Information and Modeling, 2007, 47, 1163-1170.	2.5	7
130	A Fragment-Based Scoring Function to Re-rank ATP Docking Results. International Journal of Molecular Sciences, 2007, 8, 1083-1094.	1.8	9
131	Specificity of helix packing in transmembrane dimer of the cell death factor BNIP3: A molecular modeling study. Proteins: Structure, Function and Bioinformatics, 2007, 69, 309-325.	1.5	15
132	A novel method for packing quality assessment of transmembrane α -helical domains in proteins. Biochemistry (Moscow), 2007, 72, 293-300.	0.7	0
133	Protein-Membrane Interactions: Lessons from In Silico Studies. , 2007, , 19-39.		1
134	Spatial Structure and Activity Mechanism of a Novel Spider Antimicrobial Peptide,. Biochemistry, 2006, 45, 10759-10767.	1.2	37
135	Differences in Binding Sites of Two Melatonin Receptors Help to Explain Their Selectivity to Some Melatonin Analogs: A Molecular Modeling Study. Journal of Biomolecular Structure and Dynamics, 2006, 24, 91-107.	2.0	16
136	Complementarity of hydrophobic properties in ATP-protein binding: A new criterion to rank docking solutions. Proteins: Structure, Function and Bioinformatics, 2006, 66, 388-398.	1.5	21
137	Solution of the spatial structure of dimeric transmembrane domains of proteins by heteronuclear NMR spectroscopy and molecular modeling. Biophysics (Russian Federation), 2006, 51, 23-27.	0.2	2
138	Association of transmembrane helices: what determines assembling of a dimer?. Journal of Computer-Aided Molecular Design, 2006, 20, 27-45.	1.3	23
139	Computer Simulations of Anionic Unsaturated Lipid Bilayer "A Suitable Model to Study Membrane Interactions with A Cell-Penetrating Peptide. , 2006, , 235-246.		0
140	Interaction of three-finger toxins with phospholipid membranes: comparison of S- and P-type cytotoxins. Biochemical Journal, 2005, 387, 807-815.	1.7	59
141	Role of Lipid Charge in Organization of Water/Lipid Bilayer Interface: Insights via Computer Simulations. Journal of Physical Chemistry B, 2005, 109, 15052-15059.	1.2	40
142	Effect of Lipid Composition on the "Membrane Response" Induced by a Fusion Peptide". Biochemistry, 2005, 44, 14626-14637.	1.2	31
143	Helix Interactions in Membranes: Lessons from Unrestrained Monte Carlo Simulations. Journal of Chemical Theory and Computation, 2005, 1, 1252-1264.	2.3	13
144	Peptides and Proteins in Membranes: What Can We Learn via Computer Simulations?. Current Medicinal Chemistry, 2004, 11, 2421-2442.	1.2	54

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145	The Distinct Functional Properties of the Nucleotide-binding Domain of ATP7B, the Human Copper-transporting ATPase. <i>Journal of Biological Chemistry</i> , 2004, 279, 36363-36371.	1.6	56
146	Correlation of Local Changes in the Temperature-Dependent Conformational Flexibility of Thioredoxins with Their Thermostability. <i>Russian Journal of Bioorganic Chemistry</i> , 2004, 30, 421-430.	0.3	8
147	Development of the force field parameters for phosphoimidazole and phosphohistidine. <i>Journal of Computational Chemistry</i> , 2004, 25, 1313-1321.	1.5	10
148	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. <i>Biochemical Journal</i> , 2004, 382, 293-305.	1.7	23
149	Pyrenemethyl ara-Uridine-2- ϵ -carbamate: A Strong Interstrand Excimer in the Major Groove of a DNA Duplex. <i>ChemBioChem</i> , 2003, 4, 841-847.	1.3	61
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