

# Roman G Efremov

## List of Publications by Year in descending order

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197  
papers

4,501  
citations

94433

37  
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149698

56  
g-index

205  
all docs

205  
docs citations

205  
times ranked

4198  
citing authors

#	ARTICLE	IF	CITATIONS
1	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.	3.4	189
2	PLATINUM: a web tool for analysis of hydrophobic/hydrophilic organization of biomolecular complexes. <i>Bioinformatics</i> , 2009, 25, 1201-1202.	4.1	159
3	Molecular Lipophilicity in Protein Modeling and Drug Design. <i>Current Medicinal Chemistry</i> , 2007, 14, 393-415.	2.4	128
4	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.	3.4	121
5	Surface-enhanced Raman spectroscopy of biomolecules. Part I.-water-soluble proteins, dipeptides and amino acids. <i>Journal of Raman Spectroscopy</i> , 1990, 21, 43-48.	2.5	109
6	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.	3.4	100
7	Left-Handed Dimer of EphA2 Transmembrane Domain: Helix Packing Diversity among Receptor Tyrosine Kinases. <i>Biophysical Journal</i> , 2010, 98, 881-889.	0.5	100
8	Insulin Receptor-Related Receptor as an Extracellular Alkali Sensor. <i>Cell Metabolism</i> , 2011, 13, 679-689.	16.2	92
9	PREDDIMER: a web server for prediction of transmembrane helical dimers. <i>Bioinformatics</i> , 2014, 30, 889-890.	4.1	77
10	Structural mechanism of heat-induced opening of a temperature-sensitive TRP channel. <i>Nature Structural and Molecular Biology</i> , 2021, 28, 564-572.	8.2	76
11	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.	2.6	72
12	The Role of the Invariant His-1069 in Folding and Function of the Wilson's Disease Protein, the Human Copper-transporting ATPase ATP7B. <i>Journal of Biological Chemistry</i> , 2003, 278, 13302-13308.	3.4	66
13	Antimicrobial Peptides Induce Growth of Phosphatidylglycerol Domains in a Model Bacterial Membrane. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 3108-3111.	4.6	65
14	How broadly tuned olfactory receptors equally recognize their agonists. Human OR1G1 as a test case. <i>Cellular and Molecular Life Sciences</i> , 2012, 69, 4205-4213.	5.4	64
15	A Solvent Model for Simulations of Peptides in Bilayers. I. Membrane-Promoting $\alpha$ -Helix Formation. <i>Biophysical Journal</i> , 1999, 76, 2448-2459.	0.5	63
16	Multistate Organization of Transmembrane Helical Protein Dimers Governed by the Host Membrane. <i>Journal of the American Chemical Society</i> , 2012, 134, 14390-14400.	13.7	63
17	Human copper-transporting ATPase ATP7B (the Wilson's disease protein): biochemical properties and regulation. <i>Journal of Bioenergetics and Biomembranes</i> , 2002, 34, 351-362.	2.3	61
18	Pyrenemethyl ara-Uridine-2'-carbamate: A Strong Interstrand Excimer in the Major Groove of a DNA Duplex. <i>ChemBioChem</i> , 2003, 4, 841-847.	2.6	61

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19	Interaction of three-finger toxins with phospholipid membranes: comparison of S- and P-type cytotoxins. <i>Biochemical Journal</i> , 2005, 387, 807-815.	3.7	59
20	Structure and Dynamics of Cardiotoxins. <i>Current Protein and Peptide Science</i> , 2012, 13, 570-584.	1.4	58
21	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.	3.4	56
22	Lipid-II forms potential "landing terrain" for lantibiotics in simulated bacterial membrane. <i>Scientific Reports</i> , 2013, 3, 1678.	3.3	56
23	Peptides and Proteins in Membranes: What Can We Learn via Computer Simulations?. <i>Current Medicinal Chemistry</i> , 2004, 11, 2421-2442.	2.4	54
24	Latarcins: versatile spider venom peptides. <i>Cellular and Molecular Life Sciences</i> , 2015, 72, 4501-4522.	5.4	54
25	Snake Cytotoxins Bind to Membranes via Interactions with Phosphatidylserine Head Groups of Lipids. <i>PLoS ONE</i> , 2011, 6, e19064.	2.5	53
26	Interaction between the Elastin Peptide VGVAPG and Human Elastin Binding Protein. <i>Journal of Biological Chemistry</i> , 2013, 288, 1317-1328.	3.4	50
27	Temperature-sensitive gating of TRPV1 channel as probed by atomistic simulations of its trans- and juxtamembrane domains. <i>Scientific Reports</i> , 2016, 6, 33112.	3.3	49
28	Cobra Cardiotoxins: Membrane Interactions and Pharmacological Potential. <i>Current Medicinal Chemistry</i> , 2013, 21, 270-287.	2.4	48
29	Interaction of Cardiotoxins with Membranes: A Molecular Modeling Study. <i>Biophysical Journal</i> , 2002, 83, 144-153.	0.5	46
30	New Insights into Molecular Organization of Human Neuraminidase-1: Transmembrane Topology and Dimerization Ability. <i>Scientific Reports</i> , 2016, 6, 38363.	3.3	44
31	Hydrophobic Nature of Membrane-Spanning $\alpha$ -Helical Peptides as Revealed by Monte Carlo Simulations and Molecular Hydrophobicity Potential Analysis. <i>The Journal of Physical Chemistry</i> , 1995, 99, 10658-10666.	2.9	42
32	Spatial Structure of Zervamicin IIB Bound to DPC Micelles: Implications for Voltage-Gating. <i>Biophysical Journal</i> , 2002, 82, 762-771.	0.5	42
33	Liquid but Durable: Molecular Dynamics Simulations Explain the Unique Properties of Archaeal-Like Membranes. <i>Scientific Reports</i> , 2014, 4, 7462.	3.3	42
34	Factors important for fusogenic activity of peptides: molecular modeling study of analogs of fusion peptide of influenza virus hemagglutinin. <i>FEBS Letters</i> , 1999, 462, 205-210.	2.8	40
35	Role of Lipid Charge in Organization of Water/Lipid Bilayer Interface: Insights via Computer Simulations. <i>Journal of Physical Chemistry B</i> , 2005, 109, 15052-15059.	2.6	40
36	Environmental Characteristics of Residues in Proteins: Three-Dimensional Molecular Hydrophobicity Potential Approach. <i>Journal of Biomolecular Structure and Dynamics</i> , 1993, 11, 483-507.	3.5	39

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37	A cytochrome c mutant with high electron transfer and antioxidant activities but devoid of apoptogenic effect. <i>Biochemical Journal</i> , 2002, 362, 749.	3.7	39
38	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.	2.5	39
39	Three-Dimensional Structure/Hydrophobicity of Latarcins Specifies Their Mode of Membrane Activity. <i>Biochemistry</i> , 2008, 47, 3525-3533.	2.5	38
40	Linker and/or transmembrane regions of influenza A/Group-1, A/Group-2, and type B virus hemagglutinins are packed differently within trimers. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2011, 1808, 1843-1854.	2.6	38
41	Surface-enhanced Raman spectroscopy of biomolecules. Part II. Application of short- and long-range components of SERS to the study of the structure and function of membrane proteins. <i>Journal of Raman Spectroscopy</i> , 1990, 21, 49-53.	2.5	37
42	Spatial Structure and Activity Mechanism of a Novel Spider Antimicrobial Peptide. <i>Biochemistry</i> , 2006, 45, 10759-10767.	2.5	37
43	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.	3.4	37
44	Dimeric Structure of the Transmembrane Domain of Glycophorin A in Lipidic and Detergent Environments. <i>Acta Naturae</i> , 2011, 3, 90-98.	1.7	37
45	A Solvent Model for Simulations of Peptides in Bilayers. II. Membrane-Spanning $\alpha$ -Helices. <i>Biophysical Journal</i> , 1999, 76, 2460-2471.	0.5	36
46	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.	2.6	36
47	N-terminal amphipathic helix as a trigger of hemolytic activity in antimicrobial peptides: A case study in latarcins. <i>FEBS Letters</i> , 2009, 583, 2425-2428.	2.8	34
48	Structure elucidation of dimeric transmembrane domains of bitopic proteins. <i>Cell Adhesion and Migration</i> , 2010, 4, 284-298.	2.7	34
49	Nontrivial Behavior of Water in the Vicinity and Inside Lipid Bilayers As Probed by Molecular Dynamics Simulations. <i>ACS Nano</i> , 2013, 7, 9428-9442.	14.6	34
50	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.	3.3	34
51	Effect of Lipid Composition on the Membrane Response Induced by a Fusion Peptide. <i>Biochemistry</i> , 2005, 44, 14626-14637.	2.5	31
52	Specific Membrane Binding of Neurotoxin II Can Facilitate Its Delivery to Acetylcholine Receptor. <i>Biophysical Journal</i> , 2009, 97, 2089-2097.	0.5	31
53	Modular Organization of $\alpha$ -Toxins from Scorpion Venom Mirrors Domain Structure of Their Targets, Sodium Channels. <i>Journal of Biological Chemistry</i> , 2013, 288, 19014-19027.	3.4	31
54	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 <sup>+</sup> , K <sup>+</sup> -ATPase. <i>The Protein Journal</i> , 1992, 11, 665-675.	1.1	30

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55	Effect of hydrophobic environment on the resonance Raman spectra of tryptophan residues in proteins. <i>Journal of Raman Spectroscopy</i> , 1992, 23, 69-73.	2.5	29
56	Spatial structure of the M2 transmembrane segment of the nicotinic acetylcholine receptor $\hat{\alpha}$ -subunit. <i>FEBS Letters</i> , 1999, 457, 117-121.	2.8	28
57	Deciphering Fine Molecular Details of Proteins' Structure and Function with a Protein Surface Topography (PST) Method. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 1189-1199.	5.4	28
58	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.	2.4	28
59	Kalium 2.0, a comprehensive database of polypeptide ligands of potassium channels. <i>Scientific Data</i> , 2019, 6, 73.	5.3	28
60	Differentiated analysis of the secondary structure of hydrophilic and hydrophobic regions in $\hat{\alpha}$ - and $\hat{\beta}$ -subunits of Na <sup>+</sup> ,K <sup>+</sup> -ATPase by Raman spectroscopy. <i>FEBS Letters</i> , 1988, 227, 235-239.	2.8	27
61	Atomic-scale lateral heterogeneity and dynamics of two-component lipid bilayers composed of saturated and unsaturated phosphatidylcholines. <i>Soft Matter</i> , 2011, 7, 2569.	2.7	27
62	Elastic fibers and elastin receptor complex: Neuraminidase-1 takes the center stage. <i>Matrix Biology</i> , 2019, 84, 57-67.	3.6	27
63	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.	3.7	23
64	Association of transmembrane helices: what determines assembling of a dimer?. <i>Journal of Computer-Aided Molecular Design</i> , 2006, 20, 27-45.	2.9	23
65	Homology modeling of MT1 and MT2 receptors. <i>European Journal of Medicinal Chemistry</i> , 2008, 43, 1926-1944.	5.5	23
66	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.	2.6	23
67	High-Affinity $\hat{\alpha}$ -Conotoxin PnIA Analogs Designed on the Basis of the Protein Surface Topography Method. <i>Scientific Reports</i> , 2016, 6, 36848.	3.3	23
68	Dimeric structure of the transmembrane domain of glycophorin a in lipidic and detergent environments. <i>Acta Naturae</i> , 2011, 3, 90-8.	1.7	23
69	The chromophore-binding site of bacteriorhodopsin. Resonance Raman and surface-enhanced resonance Raman spectroscopy and quantum chemical study. <i>Journal of Biosciences</i> , 1985, 8, 363-374.	1.1	22
70	Complementarity of hydrophobic properties in ATP-protein binding: A new criterion to rank docking solutions. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006, 66, 388-398.	2.6	21
71	Adaptable Lipid Matrix Promotes Protein-Protein Association in Membranes. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4415-4426.	5.3	21
72	Environmental and dynamic effects explain how nisin captures membrane-bound lipid II. <i>Scientific Reports</i> , 2020, 10, 8821.	3.3	21

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73	Transmembrane Peptides as Inhibitors of Protein-Protein Interactions: An Efficient Strategy to Target Cancer Cells?. <i>Frontiers in Oncology</i> , 2020, 10, 519.	2.8	21
74	Role of Dimerization Efficiency of Transmembrane Domains in Activation of Fibroblast Growth Factor Receptor 3. <i>Journal of the American Chemical Society</i> , 2013, 135, 8105-8108.	13.7	20
75	KV1.2 channel-specific blocker from <i>Mesobuthus eupeus</i> scorpion venom: Structural basis of selectivity. <i>Neuropharmacology</i> , 2018, 143, 228-238.	4.1	20
76	Atomic Solvation Parameters for Proteins in a Membrane Environment. Application to Transmembrane $\alpha$ -Helices. <i>Journal of Biomolecular Structure and Dynamics</i> , 1997, 15, 1-18.	3.5	19
77	Recent Advances in Computational Modeling of $\alpha$ -Helical Membrane-Active Peptides. <i>Current Protein and Peptide Science</i> , 2012, 13, 644-657.	1.4	19
78	Implicit two-phase solvation model as a tool to assess conformation and energetics of proteins in membrane-mimetic media. <i>Theoretical Chemistry Accounts</i> , 2001, 106, 48-54.	1.4	18
79	The X-ray structure of <i>Salmonella typhimurium</i> uridine nucleoside phosphorylase complexed with 2,2'-anhydrouridine, phosphate and potassium ions at 1.86 Å resolution. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010, 66, 51-60.	2.5	18
80	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.	1.6	18
81	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
82	Binding of monovalent cations induces large changes in the secondary structure of Na <sup>+</sup> ,K <sup>+</sup> -ATPase as probed by Raman spectroscopy. <i>FEBS Letters</i> , 1988, 236, 235-239.	2.8	16
83	Study of ATP binding in the active site of Na <sup>+</sup> ,K <sup>+</sup> -ATPase as probed by ultraviolet resonance Raman spectroscopy. <i>FEBS Letters</i> , 1990, 260, 257-260.	2.8	16
84	Differences in Binding Sites of Two Melatonin Receptors Help to Explain Their Selectivity to Some Melatonin Analogs: A Molecular Modeling Study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2006, 24, 91-107.	3.5	16
85	Specificity of helix packing in transmembrane dimer of the cell death factor BNIP3: A molecular modeling study. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 69, 309-325.	2.6	15
86	Cardiotoxins: Functional Role of Local Conformational Changes. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 2799-2810.	5.4	15
87	Normal coordinate treatment of 1-methylthymine in the crystalline state: Use of the ultraviolet resonance Raman intensities to improve the vibrational force field. <i>Spectrochimica Acta Part A: Molecular Spectroscopy</i> , 1994, 50, 961-971.	0.1	14
88	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.	5.4	14
89	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 <sup>+</sup> , K <sup>+</sup> -ATPase. <i>The Protein Journal</i> , 1992, 11, 699-708.	1.1	13
90	Helix Interactions in Membranes: Lessons from Unrestrained Monte Carlo Simulations. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 1252-1264.	5.3	13

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91	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.	3.5	13
92	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.	3.4	13
93	Retinal Schiff base position relative to the surfaces of photoreceptor disk. <i>FEBS Letters</i> , 1987, 213, 113-118.	2.8	12
94	Structural, dynamic, and functional aspects of helix association in membranes. <i>Advances in Protein Chemistry and Structural Biology</i> , 2011, 83, 129-161.	2.3	12
95	Dynamic clustering of lipids in hydrated two-component membranes: results of computer modeling and putative biological impact. <i>Journal of Biomolecular Structure and Dynamics</i> , 2013, 31, 87-95.	3.5	12
96	Amino acid residue: is it structural or functional?. <i>FEBS Letters</i> , 1995, 375, 162-166.	2.8	11
97	Hydrophobic organization of Î±-helix membrane bundle in bacteriorhodopsin. <i>The Protein Journal</i> , 1996, 15, 63-76.	1.1	11
98	Docking of ATP to Ca-ATPase:â€” Considering Protein Domain Motions. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 1171-1181.	5.4	11
99	Ligand-specific scoring functions: improved ranking of docking solutions. <i>SAR and QSAR in Environmental Research</i> , 2008, 19, 91-99.	2.2	11
100	Computer simulations and modeling-assisted ToxR screening in deciphering 3D structures of transmembrane Î±-helical dimers: ephrin receptor A1. <i>Physical Biology</i> , 2010, 7, 016014.	1.8	11
101	Complex approach for analysis of snake venom Î±-neurotoxins binding to HAP, the high-affinity peptide. <i>Scientific Reports</i> , 2020, 10, 3861.	3.3	11
102	Transmembrane Peptides as a New Strategy to Inhibit Neuraminidase-1 Activation. <i>Frontiers in Cell and Developmental Biology</i> , 2020, 8, 611121.	3.7	11
103	Quantitative Treatment of UV Resonance Raman Spectra of Biological Molecules: Application to the Study of Membrane-Bound Proteins. <i>Applied Spectroscopy</i> , 1991, 45, 272-278.	2.2	10
104	Development of the force field parameters for phosphoimidazole and phosphohistidine. <i>Journal of Computational Chemistry</i> , 2004, 25, 1313-1321.	3.3	10
105	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.	2.6	10
106	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.	3.4	10
107	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.	3.7	10
108	COMPUTER SIMULATIONS OF MEMBRANE-LYTIC PEPTIDES: PERSPECTIVES IN DRUG DESIGN. <i>Journal of Bioinformatics and Computational Biology</i> , 2007, 05, 611-626.	0.8	9

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109	A Fragment-Based Scoring Function to Re-rank ATP Docking Results. <i>International Journal of Molecular Sciences</i> , 2007, 8, 1083-1094.	4.1	9
110	A Single Missense Mutation in a Coiled-Coil Domain of <i>Escherichia coli</i> Ribosomal Protein S2 Confers a Thermosensitive Phenotype That Can Be Suppressed by Ribosomal Protein S1. <i>Journal of Bacteriology</i> , 2013, 195, 95-104.	2.2	9
111	libxtc: an efficient library for reading XTC-compressed MD trajectory data. <i>BMC Research Notes</i> , 2021, 14, 124.	1.4	9
112	Molecular Dynamics Insight into the Lipid II Recognition by Type A Lantibiotics: Nisin, Epidermin, and Gallidermin. <i>Micromachines</i> , 2021, 12, 1169.	2.9	9
113	Anionic Lipids: Determinants of Binding Cytotoxins from Snake Venom on the Surface of Cell Membranes. <i>Acta Naturae</i> , 2010, 2, 88-95.	1.7	9
114	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 <sup>+</sup> , K <sup>+</sup> -ATPase. <i>The Protein Journal</i> , 1993, 12, 143-152.	1.1	8
115	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.	1.0	8
116	Analysis of hydrophobic interactions of antagonists with the beta2-adrenergic receptor. SAR and QSAR in Environmental Research, 2010, 21, 37-55.	2.2	8
117	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.	2.3	8
118	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.	2.5	8
119	Why human anti-Gal $\beta$ 1 $\rightarrow$ 4Gal $\beta$ 2 $\rightarrow$ 4Glc natural antibodies do not recognize the trisaccharide on erythrocyte membrane? Molecular dynamics and immunochemical investigation. <i>Molecular Immunology</i> , 2017, 90, 87-97.	2.2	8
120	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.	3.0	8
121	Dielectric-Dependent Strength of Interlipid Hydrogen Bonding in Biomembranes: Model Case Study. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2765-2775.	5.4	8
122	Atomistic mechanism of the constitutive activation of PDGFRA via its transmembrane domain. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2019, 1863, 82-95.	2.4	8
123	Tuning Scorpion Toxin Selectivity: Switching From KV1.1 to KV1.3. <i>Frontiers in Pharmacology</i> , 2020, 11, 1010.	3.5	8
124	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.	6.4	8
125	Architecture of the Sodium Pump Molecule.. <i>Annals of the New York Academy of Sciences</i> , 1992, 671, 134-146.	3.8	7
126	Recognition of transmembrane $\alpha$ -helical segments with environmental profiles. <i>Protein Engineering, Design and Selection</i> , 1996, 9, 253-263.	2.1	7



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127	Molecular Modeling of HIV-1 Coreceptor CCR5 and Exploring of Conformational Space of its Extracellular Domain in Molecular Dynamics Simulation. <i>Journal of Biomolecular Structure and Dynamics</i> , 1998, 16, 77-90.	3.5	7
128	Monte Carlo simulations of voltage-driven translocation of a signal sequence. <i>FEBS Letters</i> , 2002, 526, 97-100.	2.8	7
129	Method To Assess Packing Quality of Transmembrane $\alpha$ -Helices in Proteins. 1. Parametrization Using Structural Data. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 1150-1162.	5.4	7
130	Method To Assess Packing Quality of Transmembrane $\alpha$ -Helices in Proteins. 2. Validation by $\alpha$ -Correct vs Misleading $\alpha$ -Test. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 1163-1170.	5.4	7
131	Interaction of linear cationic peptides with phospholipid membranes and polymers of sialic acid. <i>Biochemistry (Moscow)</i> , 2014, 79, 459-468.	1.5	7
132	Improving therapeutic potential of antibacterial spider venom peptides: coarse-grain molecular dynamics guided approach. <i>Future Medicinal Chemistry</i> , 2018, 10, 2309-2322.	2.3	7
133	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
134	All-d-Enantiomeric Peptide D3 Designed for Alzheimer's Disease Treatment Dynamically Interacts with Membrane-Bound Amyloid- $\beta$ Precursors. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 16464-16479.	6.4	7
135	Detailed Assessment of Spatial Hydrophobic and Electrostatic Properties of 2D NMR-Derived Models of Neurotoxin II. <i>Journal of Biomolecular Structure and Dynamics</i> , 1995, 12, 971-991.	3.5	6
136	Cobra cytotoxins: determinants of antibacterial activity. <i>Mendeleev Communications</i> , 2015, 25, 70-71.	1.6	6
137	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.	2.6	6
138	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.	4.1	6
139	Stepwise Insertion of Cobra Cardiotoxin CT2 into a Lipid Bilayer Occurs as an Interplay of Protein and Membrane $\alpha$ -Dynamic Molecular Portraits. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 385-399.	5.4	6
140	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
141	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.	3.4	6
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