Artem Cherkasov

List of Publications by Year
in descending order

115 papers	8,455 citations	66234 42 h-index	48187 88 g-index
122 all docs	122 docs citations	122 times ranked	10613 citing authors

#	Article	IF	Citations
1	QSAR Modeling: Where Have You Been? Where Are You Going To?. Journal of Medicinal Chemistry, 2014, 57, 4977-5010.	2.9	1,401
2	The value of antimicrobial peptides in the age of resistance. Lancet Infectious Diseases, The, 2020, 20, e216-e230.	4.6	573
3	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	18.7	427
4	Rapid Identification of Potential Inhibitors of SARSâ€CoVâ€2 Main Protease by Deep Docking of 1.3â€...Billion Compounds. Molecular Informatics, 2020, 39, e2000028.	1.4	398
5	Use of Artificial Intelligence in the Design of Small Peptide Antibiotics Effective against a Broad Spectrum of Highly Antibiotic-Resistant Superbugs. ACS Chemical Biology, 2009, 4, 65-74.	1.6	303
6	Combinatorial QSAR Modeling of Chemical Toxicants Tested against Tetrahymena pyriformis. Journal of Chemical Information and Modeling, 2008, 48, 766-784.	2.5	258
7	Identification of Novel Antibacterial Peptides by Chemoinformatics and Machine Learning. Journal of Medicinal Chemistry, 2009, 52, 2006-2015.	2.9	250
8	SimBoost: a read-across approach for predicting drugâ€“target binding affinities using gradient boosting machines. Journal of Cheminformatics, 2017, 9, 24.	2.8	227
9	Applicability Domains for Classification Problems: Benchmarking of Distance to Models for Ames Mutagenicity Set. Journal of Chemical Information and Modeling, 2010, 50, 2094-2111.	2.5	202
10	Deep Docking: A Deep Learning Platform for Augmentation of Structure Based Drug Discovery. ACS Central Science, 2020, 6, 939-949.	5.3	195
11	Functional analysis of androgen receptor mutations that confer anti-androgen resistance identified in circulating cell-free DNA from prostate cancer patients. Genome Biology, 2016, 17, 10.	3.8	165
12	Crystallographic structure of wild-type SARS-CoV-2 main protease acyl-enzyme intermediate with physiological C-terminal autoprocessing site. Nature Communications, 2020, 11, 5877.	5.8	141
13	Targeting the Binding Function 3 (BF3) Site of the Human Androgen Receptor through Virtual Screening.. Journal of Medicinal Chemistry, 2011, 54, 8563-8573.	2.9	136
14	A critical overview of computational approaches employed for COVID-19 drug discovery. Chemical Society Reviews, 2021, 50, 9121-9151.	18.7	128
15	Evidence That Plant-Like Genes in Chlamydia Species Reflect an Ancestral Relationship between Chlamydiaceae, Cyanobacteria, and the Chloroplast. Genome Research, 2002, 12, 1159-1167.	2.4	114
16	Therapeutic Inhibition of Myc in Cancer. Structural Bases and Computer-Aided Drug Discovery Approaches. International Journal of Molecular Sciences, 2019, 20, 120.	1.8	109
17	Selectively Targeting the DNA-binding Domain of the Androgen Receptor as a Prospective Therapy for Prostate Cancer. Journal of Biological Chemistry, 2014, 289, 26417-26429.	1.6	107
18	Artificial intelligenceâ€enabled virtual screening of ultra-large chemical libraries with deep docking. Nature Protocols, 2022, 17, 672-697.	5.5	107

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19	Role of Androgen Receptor Variants in Prostate Cancer: Report from the 2017 Mission Androgen Receptor Variants Meeting. European Urology, 2018, 73, 715-723.	0.9	105
20	Discovery of Small-Molecule Inhibitors Selectively Targeting the DNA-Binding Domain of the Human Androgen Receptor. Journal of Medicinal Chemistry, 2014, 57, 6458-6467.	2.9	102
21	Toxic Colors: The Use of Deep Learning for Predicting Toxicity of Compounds Merely from Their Graphic Images. Journal of Chemical Information and Modeling, 2018, 58, 1533-1543.	2.5	101
22	Best Practices of Computer-Aided Drug Discovery: Lessons Learned from the Development of a Preclinical Candidate for Prostate Cancer with a New Mechanism of Action. Journal of Chemical Information and Modeling, 2017, 57, 1018-1028.	2.5	92
23	Inhibitors of Androgen Receptor Activation Function-2 (AF2) Site Identified through Virtual Screening. Journal of Medicinal Chemistry, 2011, 54, 6197-6205.	2.9	85
24	The mycobacterial antibiotic resistance determinant WhiB7 acts as a transcriptional activator by binding the primary sigma factor SigA (RpoV). Nucleic Acids Research, 2013, 41, 10062-10076.	6.5	83
25	Targeting the Binding Function 3 (BF3) Site of the Androgen Receptor Through Virtual Screening. 2. Development of 2-((2-phenoxyethyl) thio)-1H-benzimidazole Derivatives. Journal of Medicinal Chemistry, 2013, 56, 1136-1148.	2.9	81
26	Moving Towards Precision Urologic Oncology: Targeting Enzalutamide-resistant Prostate Cancer and Mutated Forms of the Androgen Receptor Using the Novel Inhibitor Darolutamide (ODM-201). European Urology, 2018, 73, 4-8.	0.9	75
27	The transformational role of GPU computing and deep learning in drug discovery. Nature Machine Intelligence, 2022, 4, 211-221.	8.3	73
28	Optimization of Antibacterial Peptides by Genetic Algorithms and Cheminformatics. Chemical Biology and Drug Design, 2011, 77, 48-56.	1.5	72
29	Structural analyses of sex hormone-binding globulin reveal novel ligands and function. Molecular and Cellular Endocrinology, 2010, 316, 13-23.	1.6	70
30	Molecular Analysis of the Multiple GroEL Proteins of Chlamydiae. Journal of Bacteriology, 2003, 185, 1958-1966.	1.0	63
31	ETS transcription factors as emerging drug targets in cancer. Medicinal Research Reviews, 2020, 40, 413-430.	5.0	63
32	Evaluating Different Descriptors for Model Design of Antimicrobial Peptides with Enhanced Activity Toward P. aeruginosa. Chemical Biology and Drug Design, 2007, 70, 134-142.	1.5	60
33	Identification of a Potent Antiandrogen that Targets the BF3 Site of the Androgen Receptor and Inhibits Enzalutamide-Resistant Prostate Cancer. Chemistry and Biology, 2014, 21, 1476-1485.	6.2	59
34	Scaffold Tailoring by a Newly Detected Pictetâ€“Spenglerase Activity of Strictosidine Synthase: From the Common Tryptoline Skeleton to the Rare Piperazino-indole Framework. Journal of the American Chemical Society, 2012, 134, 1498-1500.	6.6	57
35	The use of Gene Ontology terms for predicting highly-connected 'hub' nodes in protein-protein interaction networks. BMC Systems Biology, 2008, 2, 80.	3.0	55
36	Mapping the Protein Interaction Network in Methicillin-Resistant Staphylococcus aureus. Journal of Proteome Research, 2011, 10, 1139-1150.	1.8	55

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37	Identification of novel host defense peptides and the absence of Î±â€defensins in the bovine genome. Proteins: Structure, Function and Bioinformatics, 2008, 73, 420-430.	1.5	53
38	Discovery of 1H-Indole-2-carboxamides as Novel Inhibitors of the Androgen Receptor Binding Function 3 (BF3). Journal of Medicinal Chemistry, 2014, 57, 6867-6872.	2.9	53
39	Targeting Alternative Sites on the Androgen Receptor to Treat Castration-Resistant Prostate Cancer. International Journal of Molecular Sciences, 2013, 14, 12496-12519.	1.8	51
40	Comparative QSAR- and Fragments Distribution Analysis of Drugs, Druglikes, Metabolic Substances, and Antimicrobial Compounds. Journal of Chemical Information and Modeling, 2006, 46, 2167-2182.	2.5	50
41	Application of â€˜Inductiveâ€™ QSAR Descriptors for Quantification of Antibacterial Activity of Cationic Polypeptides. Molecules, 2004, 9, 1034-1052.	1.7	49
42	Luteolin is a novel p90 ribosomal S6 kinase (RSK) inhibitor that suppresses Notch4 signaling by blocking the activation of Y-box binding protein-1 (YB-1). Oncotarget, 2013, 4, 329-345.	0.8	49
43	Selectively targeting the dimerization interface of human androgen receptor with small-molecules to treat castration-resistant prostate cancer. Cancer Letters, 2018, 437, 35-43.	3.2	44
44	Inductive QSAR Descriptors. Distinguishing Compounds with Antibacterial Activity by Artificial Neural Networks. International Journal of Molecular Sciences, 2005, 6, 63-86.	1.8	43
45	Identification of Pyruvate Kinase in Methicillin-Resistant Staphylococcus aureus as a Novel Antimicrobial Drug Target. Antimicrobial Agents and Chemotherapy, 2011, 55, 2042-2053.	1.4	42
46	Progressive Docking:Â A Hybrid QSAR/Docking Approach for Accelerating In Silico High Throughput Screening. Journal of Medicinal Chemistry, 2006, 49, 7466-7478.	2.9	41
47	Successful in Silico Discovery of Novel Nonsteroidal Ligands for Human Sex Hormone Binding Globulin. Journal of Medicinal Chemistry, 2005, 48, 3203-3213.	2.9	40
48	Androgen receptor plasticity and its implications for prostate cancer therapy. Cancer Treatment Reviews, 2019, 81, 101871.	3.4	40
49	Molecular cloning, biochemical and structural analysis of elongation factor-1Î± from Leishmania donovani: comparison with the mammalian homologue. Biochemical and Biophysical Research Communications, 2003, 302, 646-652.	1.0	39
50	An Updated Steroid Benchmark Set and Its Application in the Discovery of Novel Nanomolar Ligands of Sex Hormone-Binding Globulin. Journal of Medicinal Chemistry, 2008, 51, 2047-2056.	2.9	39
51	A New Method for Estimation of Homolytic Câ˜H Bond Dissociation Enthalpies. Journal of Chemical Information and Computer Sciences, 2000, 40, 1222-1226.	2.8	38
52	Computer-aided drug discovery of Myc-Max inhibitors as potential therapeutics for prostate cancer. European Journal of Medicinal Chemistry, 2018, 160, 108-119.	2.6	38
53	Discovery and characterization of small molecules targeting the DNA-binding ETS domain of ERG in prostate cancer. Oncotarget, 2017, 8, 42438-42454.	0.8	37
54	Ivermectin inhibits HSP27 and potentiates efficacy of oncogene targeting in tumor models. Journal of Clinical Investigation, 2019, 130, 699-714.	3.9	36

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55	Automated discovery of noncovalent inhibitors of SARS-CoV-2 main protease by consensus Deep Docking of 40 billion small molecules. Chemical Science, 2021, 12, 15960-15974.	3.7	36
56	Carbonâ^'Oxygen Bond Dissociation Enthalpies in Peroxyl Radicals. Journal of Physical Chemistry A, 2000, 104, 915-921.	1.1	33
57	Towards Better BBB Passage Prediction Using an Extensive and Curated Data Set. Molecular Informatics, 2015, 34, 308-330.	1.4	33
58	Computer-Aided Ligand Discovery for Estrogen Receptor Alpha. International Journal of Molecular Sciences, 2020, 21, 4193.	1.8	33
59	Identification of Novel Androgen Receptor Antagonists Using Structure- and Ligand-Based Methods. Journal of Chemical Information and Modeling, 2013, 53, 123-130.	2.5	32
60	A phosphorylation site in the Toll-like receptor 5 TIR domain is required for inflammatory signalling in response to flagellin. Biochemical and Biophysical Research Communications, 2007, 352, 936-941.	1.0	31
61	Indel-based targeting of essential proteins in human pathogens that have close host orthologue(s): Discovery of selective inhibitors for Leishmania donovani elongation factor-1Î±. Proteins: Structure, Function and Bioinformatics, 2007, 67, 53-64.	1.5	29
62	Computer-Aided Discovery of Small Molecules Targeting the RNA Splicing Activity of hnRNP A1 in Castration-Resistant Prostate Cancer. Molecules, 2019, 24, 763.	1.7	29
63	Substituent Effects on Thermochemical Properties of Free Radicals. New Substituent Scales for C-Centered Radicals. Journal of Chemical Information and Computer Sciences, 1998, 38, 1151-1156.	2.8	28
64	Orphan nuclear receptors as drug targets for the treatment of prostate and breast cancers. Cancer Treatment Reviews, 2014, 40, 1137-1152.	3.4	26
65	A Non-Synonymous Coding Variant (L616F) in the TLR5 Gene Is Potentially Associated with Crohn's Disease and Influences Responses to Bacterial Flagellin. PLoS ONE, 2013, 8, e61326.	1.1	26
66	In silico identification of anthropogenic chemicals as ligands of zebrafish sex hormone binding globulin. Toxicology and Applied Pharmacology, 2009, 234, 47-57.	1.3	25
67	The Effect of Insertions and Deletions on Wirings in Protein-Protein Interaction Networks: A Large-Scale Study. Journal of Computational Biology, 2009, 16, 159-167.	0.8	25
68	Optimization and structureâ€“activity relationships of a series of potent inhibitors of methicillin-resistant Staphylococcus aureus (MRSA) pyruvate kinase as novel antimicrobial agents. Bioorganic and Medicinal Chemistry, 2012, 20, 7069-7082.	1.4	25
69	Inductive Electronegativity Scale. Iterative Calculation of Inductive Partial Charges. Journal of Chemical Information and Computer Sciences, 2003, 43, 2039-2047.	2.8	24
70	Targeting Binding Function-3 of the Androgen Receptor Blocks Its Co-Chaperone Interactions, Nuclear Translocation, and Activation. Molecular Cancer Therapeutics, 2016, 15, 2936-2945.	1.9	24
71	Cheminformatics-Driven Discovery of Selective, Nanomolar Inhibitors for Staphylococcal Pyruvate Kinase. ACS Chemical Biology, 2012, 7, 350-359.	1.6	23
72	Characterization of a New Class of Androgen Receptor Antagonists with Potential Therapeutic Application in Advanced Prostate Cancer. Molecular Cancer Therapeutics, 2013, 12, 2425-2435.	1.9	22

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73	Bypassing Drug Resistance Mechanisms of Prostate Cancer with Small Molecules that Target Androgen Receptorâ€“Chromatin Interactions. Molecular Cancer Therapeutics, 2017, 16, 2281-2291.	1.9	22
74	Strictosidine Synthase Triggered Enantioselective Synthesis of N-Substituted (S)-3,14,18,19-Tetrahydroangustines as Novel Topoisomerase I Inhibitors. ACS Chemical Biology, 2017, 12, 3086-3092.	1.6	22
75	DeepCOP: deep learning-based approach to predict gene regulating effects of small molecules. Bioinformatics, 2020, 36, 813-818.	1.8	21
76	Selective targeting of indel-inferred differences in spatial structures of highly homologous proteins. Proteins: Structure, Function and Bioinformatics, 2005, 58, 950-954.	1.5	20
77	Large-scale survey for potentially targetable indels in bacterial and protozoan proteins. Proteins: Structure, Function and Bioinformatics, 2005, 62, 371-380.	1.5	20
78	Can â€˜Bacterial-Metabolite-Likeness' Model Improve Odds of â€˜in Silico' Antibiotic Discovery?. Journal of Chemical Information and Modeling, 2006, 46, 1214-1222.	2.5	20
79	Molecular architecture of leishmania EF-1Î± reveals a novel site that may modulate protein translation: A possible target for drug development. Biochemical and Biophysical Research Communications, 2007, 356, 886-892.	1.0	20
80	In silico discovery and validation of potent small-molecule inhibitors targeting the activation function 2 site of human oestrogen receptor Î±. Breast Cancer Research, 2015, 17, 27.	2.2	20
81	Interleukin-10 and Small Molecule SHIP1 Allosteric Regulators Trigger Anti-inflammatory Effects through SHIP1/STAT3 Complexes. IScience, 2020, 23, 101433.	1.9	20
82	Drugging the â€˜undruggableâ€™. Therapeutic targeting of proteinâ€“DNA interactions with the use of computer-aided drug discovery methods. Drug Discovery Today, 2021, 26, 2660-2679.	3.2	20
83	Discovery of New Catalytic Topoisomerase II Inhibitors for Anticancer Therapeutics. Frontiers in Oncology, 2020, 10, 633142.	1.3	19
84	Impact of Two Novel Mutations on the Structure and Function of Human Myeloperoxidase. Journal of Biological Chemistry, 2007, 282, 27994-28003.	1.6	18
85	Using Molecular Docking, 3D-QSAR, and Cluster Analysis for Screening Structurally Diverse Data Sets of Pharmacological Interest. Journal of Chemical Information and Modeling, 2008, 48, 2054-2065.	2.5	18
86	Androgen receptor transcriptionally regulates semaphorin 3C in a GATA2-dependent manner. Oncotarget, 2017, 8, 9617-9633.	0.8	18
87	Substituent Effects on Thermochemical Properties of C-, N-, O-, and S-Centered Radicals. Physical Interpretation of Substituent Effects. Journal of Chemical Information and Computer Sciences, 1999, 39, 1057-1063.	2.8	17
88	Development of Novel Inhibitors Targeting the D-Box of the DNA Binding Domain of Androgen Receptor. International Journal of Molecular Sciences, 2021, 22, 2493.	1.8	17
89	Comprehensive Consensus Analysis of SARS-CoV-2 Drug Repurposing Campaigns. Journal of Chemical Information and Modeling, 2021, 61, 3771-3788.	2.5	17
90	Cheminformatics Modeling of Adverse Drug Responses by Clinically Relevant Mutants of Human Androgen Receptor. Journal of Chemical Information and Modeling, 2016, 56, 2507-2516.	2.5	16

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91	Identification and characterization of small molecule inhibitors of the ubiquitin ligases Siah1/2 in melanoma and prostate cancer cells. Cancer Letters, 2019, 449, 145-162.	3.2	16
92	Development of an Androgen Receptor Inhibitor Targeting the N-Terminal Domain of Androgen Receptor for Treatment of Castration Resistant Prostate Cancer. Cancers, 2021, 13, 3488.	1.7	16
93	Small molecule-induced degradation of the full length and V7 truncated variant forms of human androgen receptor. European Journal of Medicinal Chemistry, 2018, 157, 1164-1173.	2.6	15
94	The Use of Methods of Computer-Aided Drug Discovery in the Development of Topoisomerase II Inhibitors: Applications and Future Directions. Journal of Chemical Information and Modeling, 2020, 60, 3703-3721.	2.5	15
95	SPARC/SFN interaction, suppresses type I collagen in dermal fibroblasts. Journal of Cellular Biochemistry, 2012, 113, 2622-2632.	1.2	14
96	Dual-Inhibitors of N-Myc and AURKA as Potential Therapy for Neuroendocrine Prostate Cancer. International Journal of Molecular Sciences, 2020, 21, 8277.	1.8	14
97	â€˜Inductive' Charges on Atoms in Proteins:Â Comparative Docking with the Extended Steroid Benchmark Set and Discovery of a Novel SHBG Ligand. Journal of Chemical Information and Modeling, 2005, 45, 1842-1853.	2.5	13
98	20(S)-protopanaxadiol regio-selectively targets androgen receptor: anticancer effects in castration-resistant prostate tumors. Oncotarget, 2018, 9, 20965-20978.	0.8	12
99	Targeting Semaphorin 3C in Prostate Cancer With Small Molecules. Journal of the Endocrine Society, 2018, 2, 1381-1394.	0.1	10
100	Computer-Aided Discovery of Small Molecule Inhibitors of Transcriptional Activity of TLX (NR2E1) Nuclear Receptor. Molecules, 2018, 23, 2967.	1.7	9
101	Benzothiophenone Derivatives Targeting Mutant Forms of Estrogen Receptor-Î± in Hormone-Resistant Breast Cancers. International Journal of Molecular Sciences, 2018, 19, 579.	1.8	9
102	Development of 2-(5,6,7-Trifluoro-1H-Indol-3-yl)-quinoline-5-carboxamide as a Potent, Selective, and Orally Available Inhibitor of Human Androgen Receptor Targeting Its Binding Function-3 for the Treatment of Castration-Resistant Prostate Cancer. Journal of Medicinal Chemistry, 2021, 64, 14968-14982.	2.9	9
103	Structural characterization of genomes by large scale sequence-structure threading: application of reliability analysis in structural genomics. BMC Bioinformatics, 2004, 5, 101.	1.2	8
104	Cheminformatics Driven Development of Novel Therapies for Drug Resistant Prostate Cancer. Molecular Informatics, 2018, 37, e1800043.	1.4	8
105	Development of VPC-70619, a Small-Molecule N-Myc Inhibitor as a Potential Therapy for Neuroendocrine Prostate Cancer. International Journal of Molecular Sciences, 2022, 23, 2588.	1.8	7
106	Computer-Aided Discovery of Small Molecule Inhibitors of Thymocyte Selection-Associated High Mobility Group Box Protein (TOX) as Potential Therapeutics for Cutaneous T-Cell Lymphomas. Molecules, 2019, 24, 3459.	1.7	6
107	The Use of Sequenceâ€Derived QSPR Descriptors for Predicting Highly Connected Proteins (Hubs) in Proteinâ€“Protein Interactions. QSAR and Combinatorial Science, 2009, 28, 509-519.	1.5	5
108	Quantitative Structureâ€“Price Relationship (QS$R) Modeling and the Development of Economically Feasible Drug Discovery Projects. Journal of Chemical Information and Modeling, 2019, 59, 1306-1313.	2.5	5

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109	An approach to large scale identification of non-obvious structural similarities between proteins. BMC Bioinformatics, 2004, 5, 61.	1.2	4
110	Drug-Discovery Pipeline for Novel Inhibitors of the Androgen Receptor. Methods in Molecular Biology, 2016, 1443, 31-54.	0.4	4
111	Deep Modeling of Regulating Effects of Small Molecules on Longevity-Associated Genes. Pharmaceuticals, 2021, 14, 948.	1.7	2
112	Abstract 1070: New potent inhibitors of the androgen receptor that target its BF3 surface binding site.. Cancer Research, 2013, 73, 1070-1070.	0.4	1
113	Development of novel androgen receptor inhibitors to overcome castrate-resistant prostate cancer. , 2021, , 23-46.		0
114	COMPARATIVE QSAR ANALYSIS OF BACTERIAL, FUNGAL PLANT AND HUMAN METABOLITES. , 2006, , .		0
115	Progressive Docking - Deep Learning Based Approach for Accelerated Virtual Screening. Lecture Notes in Computer Science, 2019, , 737-740.	1.0	0