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	Artificial intelligenceâ€“enabled virtual screening of ultra-large chemical libraries with deep docking. Nature Protocols, 2022, 17, 672-697.	5.5	107
2	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
3	The transformational role of GPU computing and deep learning in drug discovery. Nature Machine Intelligence, 2022, 4, 211-221.	8.3	73
4	Development of novel androgen receptor inhibitors to overcome castrate-resistant prostate cancer. , 2021, , 23-46.		0
5	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
6	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
7	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
8	Comprehensive Consensus Analysis of SARS-CoV-2 Drug Repurposing Campaigns. Journal of Chemical Information and Modeling, 2021, 61, 3771-3788.	2.5	17
9	Deep Modeling of Regulating Effects of Small Molecules on Longevity-Associated Genes. Pharmaceuticals, 2021, 14, 948.	1.7	2
10	A critical overview of computational approaches employed for COVID-19 drug discovery. Chemical Society Reviews, 2021, 50, 9121-9151.	18.7	128
11	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
12	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
13	DeepCOP: deep learning-based approach to predict gene regulating effects of small molecules. Bioinformatics, 2020, 36, 813-818.	1.8	21
14	ETS transcription factors as emerging drug targets in cancer. Medicinal Research Reviews, 2020, 40, 413-430.	5.0	63
15	Interleukin-10 and Small Molecule SHIP1 Allosteric Regulators Trigger Anti-inflammatory Effects through SHIP1/STAT3 Complexes. IScience, 2020, 23, 101433.	1.9	20
16	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
17	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
18	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

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19	Deep Docking: A Deep Learning Platform for Augmentation of Structure Based Drug Discovery. ACS Central Science, 2020, 6, 939-949.	5.3	195
20	Computer-Aided Ligand Discovery for Estrogen Receptor Alpha. International Journal of Molecular Sciences, 2020, 21, 4193.	1.8	33
21	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
22	The value of antimicrobial peptides in the age of resistance. Lancet Infectious Diseases, The, 2020, 20, e216-e230.	4.6	573
23	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	18.7	427
24	Discovery of New Catalytic Topoisomerase II Inhibitors for Anticancer Therapeutics. Frontiers in Oncology, 2020, 10, 633142.	1.3	19
25	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
26	Androgen receptor plasticity and its implications for prostate cancer therapy. Cancer Treatment Reviews, 2019, 81, 101871.	3.4	40
27	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
28	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
29	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
30	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
31	Ivermectin inhibits HSP27 and potentiates efficacy of oncogene targeting in tumor models. Journal of Clinical Investigation, 2019, 130, 699-714.	3.9	36
32	Progressive Docking - Deep Learning Based Approach for Accelerated Virtual Screening. Lecture Notes in Computer Science, 2019, , 737-740.	1.0	0
33	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
34	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
35	Computer-Aided Discovery of Small Molecule Inhibitors of Transcriptional Activity of TLX (NR2E1) Nuclear Receptor. Molecules, 2018, 23, 2967.	1.7	9
36	Targeting Semaphorin 3C in Prostate Cancer With Small Molecules. Journal of the Endocrine Society, 2018, 2, 1381-1394.	0.1	10

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37	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
38	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
39	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
40	Cheminformatics Driven Development of Novel Therapies for Drug Resistant Prostate Cancer. Molecular Informatics, 2018, 37, e1800043.	1.4	8
41	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
42	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
43	20(S)-protopanaxadiol regio-selectively targets androgen receptor: anticancer effects in castration-resistant prostate tumors. Oncotarget, 2018, 9, 20965-20978.	0.8	12
44	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
45	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
46	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
47	SimBoost: a read-across approach for predicting drugâ€“target binding affinities using gradient boosting machines. Journal of Cheminformatics, 2017, 9, 24.	2.8	227
48	Androgen receptor transcriptionally regulates semaphorin 3C in a GATA2-dependent manner. Oncotarget, 2017, 8, 9617-9633.	0.8	18
49	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
50	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
51	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
52	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
53	Drug-Discovery Pipeline for Novel Inhibitors of the Androgen Receptor. Methods in Molecular Biology, 2016, 1443, 31-54.	0.4	4
54	Towards Better BBB Passage Prediction Using an Extensive and Curated Data Set. Molecular Informatics, 2015, 34, 308-330.	1.4	33

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55	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
56	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
57	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
58	QSAR Modeling: Where Have You Been? Where Are You Going To?. Journal of Medicinal Chemistry, 2014, 57, 4977-5010.	2.9	1,401
59	Orphan nuclear receptors as drug targets for the treatment of prostate and breast cancers. Cancer Treatment Reviews, 2014, 40, 1137-1152.	3.4	26
60	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
61	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
62	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
63	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
64	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
65	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
66	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
67	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
68	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
69	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
70	Cheminformatics-Driven Discovery of Selective, Nanomolar Inhibitors for Staphylococcal Pyruvate Kinase. ACS Chemical Biology, 2012, 7, 350-359.	1.6	23
71	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
72	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

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73	SPARC/SFN interaction, suppresses type I collagen in dermal fibroblasts. Journal of Cellular Biochemistry, 2012, 113, 2622-2632.	1.2	14
74	Inhibitors of Androgen Receptor Activation Function-2 (AF2) Site Identified through Virtual Screening. Journal of Medicinal Chemistry, 2011, 54, 6197-6205.	2.9	85
75	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
76	Optimization of Antibacterial Peptides by Genetic Algorithms and Cheminformatics. Chemical Biology and Drug Design, 2011, 77, 48-56.	1.5	72
77	Mapping the Protein Interaction Network in Methicillin-Resistant Staphylococcus aureus. Journal of Proteome Research, 2011, 10, 1139-1150.	1.8	55
78	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
79	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
80	Structural analyses of sex hormone-binding globulin reveal novel ligands and function. Molecular and Cellular Endocrinology, 2010, 316, 13-23.	1.6	70
81	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
82	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
83	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
84	Identification of Novel Antibacterial Peptides by Chemoinformatics and Machine Learning. Journal of Medicinal Chemistry, 2009, 52, 2006-2015.	2.9	250
85	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
86	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
87	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
88	Combinatorial QSAR Modeling of Chemical Toxicants Tested against Tetrahymena pyriformis. Journal of Chemical Information and Modeling, 2008, 48, 766-784.	2.5	258
89	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
90	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

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91	Impact of Two Novel Mutations on the Structure and Function of Human Myeloperoxidase. Journal of Biological Chemistry, 2007, 282, 27994-28003.	1.6	18
92	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
93	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
94	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
95	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
96	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
97	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
98	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
99	COMPARATIVE QSAR ANALYSIS OF BACTERIAL, FUNGAL PLANT AND HUMAN METABOLITES. , 2006, , .		0
100	Inductive QSAR Descriptors. Distinguishing Compounds with Antibacterial Activity by Artificial Neural Networks. International Journal of Molecular Sciences, 2005, 6, 63-86.	1.8	43
101	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
102	Large-scale survey for potentially targetable indels in bacterial and protozoan proteins. Proteins: Structure, Function and Bioinformatics, 2005, 62, 371-380.	1.5	20
103	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
104	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
105	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
106	An approach to large scale identification of non-obvious structural similarities between proteins. BMC Bioinformatics, 2004, 5, 61.	1.2	4
107	Application of â€˜Inductiveâ€™ QSAR Descriptors for Quantification of Antibacterial Activity of Cationic Polypeptides. Molecules, 2004, 9, 1034-1052.	1.7	49
108	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

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109	Inductive Electronegativity Scale. Iterative Calculation of Inductive Partial Charges. Journal of Chemical Information and Computer Sciences, 2003, 43, 2039-2047.	2.8	24
110	Molecular Analysis of the Multiple GroEL Proteins of Chlamydiae. Journal of Bacteriology, 2003, 185, 1958-1966.	1.0	63
111	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
112	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
113	Carbonâ˜Oxygen Bond Dissociation Enthalpies in Peroxyl Radicals. Journal of Physical Chemistry A, 2000, 104, 915-921.	1.1	33
114	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
115	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