Anton Simeonov

List of Publications by Year
in descending order

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58	4,347	186265 28	155660 55
papers	citations	h-index	g-index

68	68	68	7720
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quantitative high-throughput screening: A titration-based approach that efficiently identifies biological activities in large chemical libraries. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 11473-11478.	7.1	733
2	Identification of small-molecule inhibitors of Zika virus infection and induced neural cell death via a drug repurposing screen. Nature Medicine, 2016, 22, 1101-1107.	30.7	581
3	High-throughput combinatorial screening identifies drugs that cooperate with ibrutinib to kill activated B-cellâ€“like diffuse large B-cell lymphoma cells. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 2349-2354.	7.1	355
4	Modelling the Tox21 10â€‰K chemical profiles for in vivo toxicity prediction and mechanism characterization. Nature Communications, 2016, 7, 10425.	12.8	202
5	Complementarity Between a Docking and a High-Throughput Screen in Discovering New Cruzain Inhibitors. Journal of Medicinal Chemistry, 2010, 53, 4891-4905.	6.4	199
6	Selective and Cell-Active Inhibitors of the USP1/ UAF1 Deubiquitinase Complex Reverse Cisplatin Resistance in Non-small Cell Lung Cancer Cells. Chemistry and Biology, 2011, 18, 1390-1400.	6.0	183
7	Emetine inhibits Zika and Ebola virus infections through two molecular mechanisms: inhibiting viral replication and decreasing viral entry. Cell Discovery, 2018, 4, 31.	6.7	128
8	A Robotic Platform for Quantitative High-Throughput Screening. Assay and Drug Development Technologies, 2008, 6, 637-657.	1.2	126
9	Genomic and protein expression analysis reveals flap endonuclease 1 (FEN1) as a key biomarker in breast and ovarian cancer. Molecular Oncology, 2014, 8, 1326-1338.	4.6	109
10	Discovery and Optimization of Potent, Cell-Active Pyrazole-Based Inhibitors of Lactate Dehydrogenase (LDH). Journal of Medicinal Chemistry, 2017, 60, 9184-9204.	6.4	98
11	AlphaScreen-Based Assays: Ultra-High-Throughput Screening for Small-Molecule Inhibitors of Challenging Enzymes and Protein-Protein Interactions. Methods in Molecular Biology, 2016, 1439, 77-98.	0.9	96
12	Structural Basis for KDM5A Histone Lysine Demethylase Inhibition by Diverse Compounds. Cell Chemical Biology, 2016, 23, 769-781.	5.2	80
13	Synergistic and Antagonistic Drug Combinations against SARS-CoV-2. Molecular Therapy, 2021, 29, 873-885.	8.2	78
14	First Selective 12-LOX Inhibitor, ML355, Impairs Thrombus Formation and Vessel Occlusion In Vivo With Minimal Effects on Hemostasis. Arteriosclerosis, Thrombosis, and Vascular Biology, 2017, 37, 1828-1839.	2.4	76
15	Recent developments in the use of differential scanning fluorometry in protein and small molecule discovery and characterization. Expert Opinion on Drug Discovery, 2013, 8, 1071-1082.	5.0	75
16	The SARS-CoV-2 Cytopathic Effect Is Blocked by Lysosome Alkalizing Small Molecules. ACS Infectious Diseases, 2021, 7, 1389-1408.	3.8	74
17	A versatile polypharmacology platform promotes cytoprotection and viability of human pluripotent and differentiated cells. Nature Methods, 2021, 18, 528-541.	19.0	72
18	KDM4/JMJD2 Histone Demethylase Inhibitors Block Prostate Tumor Growth by Suppressing the Expression of AR and BMYB-Regulated Genes. Chemistry and Biology, 2015, 22, 1185-1196.	6.0	66

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19	Discovery of Orally Bioavailable, Quinoline-Based Aldehyde Dehydrogenase 1A1 (ALDH1A1) Inhibitors with Potent Cellular Activity. Journal of Medicinal Chemistry, 2018, 61, 4883-4903.	6.4	61
20	Assessing inhibitors of mutant isocitrate dehydrogenase using a suite of pre-clinical discovery assays. Scientific Reports, 2017, 7, 12758.	3.3	59
21	Design, Synthesis, and Biological Evaluation of Quinazolin-4-one-Based Hydroxamic Acids as Dual PI3K/HDAC Inhibitors. Journal of Medicinal Chemistry, 2020, 63, 4256-4292.	6.4	59
22	Discovery of NCT-501, a Potent and Selective Theophylline-Based Inhibitor of Aldehyde Dehydrogenase 1A1 (ALDH1A1). Journal of Medicinal Chemistry, 2015, 58, 5967-5978.	6.4	52
23	Novel Consensus Architecture To Improve Performance of Large-Scale Multitask Deep Learning QSAR Models. Journal of Chemical Information and Modeling, 2019, 59, 4613-4624.	5.4	47
24	Discovery of TMPRSS2 Inhibitors from Virtual Screening as a Potential Treatment of COVID-19. ACS Pharmacology and Translational Science, 2021, 4, 1124-1135.	4.9	40
25	Biochemical and Cellular Characterization and Inhibitor Discovery of Pseudomonas aeruginosa 15-Lipoxygenase. Biochemistry, 2016, 55, 3329-3340.	2.5	39
26	Assay Guidance Manual: Quantitative Biology and Pharmacology in Preclinical Drug Discovery. Clinical and Translational Science, 2018, 11, 461-470.	3.1	38
27	Large-Scale Modeling of Multispecies Acute Toxicity End Points Using Consensus of Multitask Deep Learning Methods. Journal of Chemical Information and Modeling, 2021, 61, 653-663.	5.4	35
28	Robotic high-throughput biomanufacturing and functional differentiation ofÂhuman pluripotent stem cells. Stem Cell Reports, 2021, 16, 3076-3092.	4.8	34
29	Canvass: A Crowd-Sourced, Natural-Product Screening Library for Exploring Biological Space. ACS Central Science, 2018, 4, 1727-1741.	11.3	32
30	Pyrazole-Based Lactate Dehydrogenase Inhibitors with Optimized Cell Activity and Pharmacokinetic Properties. Journal of Medicinal Chemistry, 2020, 63, 10984-11011.	6.4	30
31	Critical Assessment of Artificial Intelligence Methods for Prediction of hERG Channel Inhibition in the â€œBig Dataâ€•Era. Journal of Chemical Information and Modeling, 2020, 60, 6007-6019.	5.4	29
32	Synthesis and SAR studies of 5-(pyridin-4-yl)-1,3,4-thiadiazol-2-amine derivatives as potent inhibitors of Bloom helicase. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 5660-5666.	2.2	28
33	Structure-Based Engineering of Irreversible Inhibitors against Histone Lysine Demethylase KDM5A. Journal of Medicinal Chemistry, 2018, 61, 10588-10601.	6.4	28
34	Identification of ML251, a Potent Inhibitor of T. brucei and T. cruzi Phosphofructokinase. ACS Medicinal Chemistry Letters, 2014, 5, 12-17.	2.8	27
35	Mining of high throughput screening database reveals AP-1 and autophagy pathways as potential targets for COVID-19 therapeutics. Scientific Reports, 2021, 11, 6725.	3.3	25
36	A Universal and High-Throughput Proteomics Sample Preparation Platform. Analytical Chemistry, 2021, 93, 8423-8431.	6.5	24

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37	Discovery and optimization of piperazine-1-thiourea-based human phosphoglycerate dehydrogenase inhibitors. Bioorganic and Medicinal Chemistry, 2018, 26, 1727-1739.	3.0	23
38	Connecting Neuronal Cell Protective Pathways and Drug Combinations in a Huntingtonâ€™s Disease Model through the Application of Quantitative Systems Pharmacology. Scientific Reports, 2017, 7, 17803.	3.3	22
39	Concise Review: Modeling Central Nervous System Diseases Using Induced Pluripotent Stem Cells. Stem Cells Translational Medicine, 2014, 3, 1418-1428.	3.3	21
40	SCAM Detective: Accurate Predictor of Small, Colloidally Aggregating Molecules. Journal of Chemical Information and Modeling, 2020, 60, 4056-4063.	5.4	21
41	A potent and selective inhibitor targeting human and murine 12/15-LOX. Bioorganic and Medicinal Chemistry, 2016, 24, 1183-1190.	3.0	15
42	Application of niclosamide and analogs as small molecule inhibitors of Zika virus and SARS-CoV-2 infection. Bioorganic and Medicinal Chemistry Letters, 2021, 40, 127906.	2.2	15
43	Kinetic and structural investigations of novel inhibitors of human epithelial 15-lipoxygenase-2. Bioorganic and Medicinal Chemistry, 2021, 46, 116349.	3.0	15
44	Structureâ€“activity relationship studies and biological characterization of human NAD+-dependent 15-hydroxyprostaglandin dehydrogenase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 630-635.	2.2	13
45	The Toxmatrix: Chemo-Genomic Profiling Identifies Interactions That Reveal Mechanisms of Toxicity. Chemical Research in Toxicology, 2018, 31, 127-136.	3.3	12
46	Discovery and Optimization of 2H-1Î»²-Pyridin-2-one Inhibitors of Mutant Isocitrate Dehydrogenase 1 for the Treatment of Cancer. Journal of Medicinal Chemistry, 2021, 64, 4913-4946.	6.4	12
47	FEN1 Blockade for Platinum Chemo-Sensitization and Synthetic Lethality in Epithelial Ovarian Cancers. Cancers, 2021, 13, 1866.	3.7	12
48	Mapping biologically active chemical space to accelerate drug discovery. Nature Reviews Drug Discovery, 2019, 18, 83-84.	46.4	11
49	Identification of environmental chemicals that activate p53 signaling after in vitro metabolic activation. Archives of Toxicology, 2022, 96, 1975-1987.	4.2	10
50	Insights into the Action of Inhibitor Enantiomers against Histone Lysine Demethylase 5A. Journal of Medicinal Chemistry, 2018, 61, 3193-3208.	6.4	9
51	Modulation of Triple Artemisinin-Based Combination Therapy Pharmacodynamics by Plasmodium falciparum Genotype. ACS Pharmacology and Translational Science, 2020, 3, 1144-1157.	4.9	8
52	An Integrated Systems Biology Approach Identifies the Proteasome as A Critical Host Machinery for ZIKV and DENV Replication. Genomics, Proteomics and Bioinformatics, 2021, 19, 108-122.	6.9	7
53	A systems approach to enable effective team science from the internal research program of the National Center for Advancing Translational Sciences. Journal of Clinical and Translational Science, 2021, 5, e163.	0.6	6
54	Hybrid In Silico Approach Reveals Novel Inhibitors of Multiple SARS-CoV-2 Variants. ACS Pharmacology and Translational Science, 2021, 4, 1675-1688.	4.9	6

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55	Discovery and Optimization of Pyrrolopyrimidine Derivatives as Selective Disruptors of the Perinucleolar Compartment, a Marker of Tumor Progression toward Metastasis. Journal of Medicinal Chemistry, 2022, 65, 8303-8331.	6.4	4
56	Inside Cover: A Highly Potent and Selective Caspaseâ€…1 Inhibitor that Utilizes a Key 3-Cyanopropanoic Acid Moiety (ChemMedChem 5/2010). ChemMedChem, 2010, 5, 634-634.	3.2	0
57	Chemically Defined Neural Conversion of Human Pluripotent Stem Cells. Methods in Molecular Biology, 2019, 1919, 59-72.	0.9	0
58	Identification of hit compounds with anti-schistosomal activity on in vitro generated juvenile worms in cell-free medium. PLoS Neglected Tropical Diseases, 2021, 15, e0009432.	3.0	0