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	Identification of environmental chemicals that activate p53 signaling after in vitro metabolic activation. Archives of Toxicology, 2022, 96, 1975-1987.	4.2	10
2	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
3	Synergistic and Antagonistic Drug Combinations against SARS-CoV-2. Molecular Therapy, 2021, 29, 873-885.	8.2	78
4	The SARS-CoV-2 Cytopathic Effect Is Blocked by Lysosome Alkalizing Small Molecules. ACS Infectious Diseases, 2021, 7, 1389-1408.	3.8	74
5	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
6	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
7	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
8	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
9	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
10	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
11	FEN1 Blockade for Platinum Chemo-Sensitization and Synthetic Lethality in Epithelial Ovarian Cancers. Cancers, 2021, 13, 1866.	3.7	12
12	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
13	A versatile polypharmacology platform promotes cytoprotection and viability of human pluripotent and differentiated cells. Nature Methods, 2021, 18, 528-541.	19.0	72
14	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
15	A Universal and High-Throughput Proteomics Sample Preparation Platform. Analytical Chemistry, 2021, 93, 8423-8431.	6.5	24
16	Kinetic and structural investigations of novel inhibitors of human epithelial 15-lipoxygenase-2. Bioorganic and Medicinal Chemistry, 2021, 46, 116349.	3.0	15
17	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
18	Robotic high-throughput biomanufacturing and functional differentiation ofÂhuman pluripotent stem cells. Stem Cell Reports, 2021, 16, 3076-3092.	4.8	34

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19	SCAM Detective: Accurate Predictor of Small, Colloidally Aggregating Molecules. Journal of Chemical Information and Modeling, 2020, 60, 4056-4063.	5.4	21
20	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
21	Pyrazole-Based Lactate Dehydrogenase Inhibitors with Optimized Cell Activity and Pharmacokinetic Properties. Journal of Medicinal Chemistry, 2020, 63, 10984-11011.	6.4	30
22	Modulation of Triple Artemisinin-Based Combination Therapy Pharmacodynamics by Plasmodium falciparum Genotype. ACS Pharmacology and Translational Science, 2020, 3, 1144-1157.	4.9	8
23	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
24	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
25	Chemically Defined Neural Conversion of Human Pluripotent Stem Cells. Methods in Molecular Biology, 2019, 1919, 59-72.	0.9	0
26	Mapping biologically active chemical space to accelerate drug discovery. Nature Reviews Drug Discovery, 2019, 18, 83-84.	46.4	11
27	Discovery and optimization of piperazine-1-thiourea-based human phosphoglycerate dehydrogenase inhibitors. Bioorganic and Medicinal Chemistry, 2018, 26, 1727-1739.	3.0	23
28	Insights into the Action of Inhibitor Enantiomers against Histone Lysine Demethylase 5A. Journal of Medicinal Chemistry, 2018, 61, 3193-3208.	6.4	9
29	The Toxmatrix: Chemo-Genomic Profiling Identifies Interactions That Reveal Mechanisms of Toxicity. Chemical Research in Toxicology, 2018, 31, 127-136.	3.3	12
30	Canvass: A Crowd-Sourced, Natural-Product Screening Library for Exploring Biological Space. ACS Central Science, 2018, 4, 1727-1741.	11.3	32
31	Structure-Based Engineering of Irreversible Inhibitors against Histone Lysine Demethylase KDM5A. Journal of Medicinal Chemistry, 2018, 61, 10588-10601.	6.4	28
32	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
33	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
34	Assay Guidance Manual: Quantitative Biology and Pharmacology in Preclinical Drug Discovery. Clinical and Translational Science, 2018, 11, 461-470.	3.1	38
35	Assessing inhibitors of mutant isocitrate dehydrogenase using a suite of pre-clinical discovery assays. Scientific Reports, 2017, 7, 12758.	3.3	59
36	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

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37	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
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	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
40	Structural Basis for KDM5A Histone Lysine Demethylase Inhibition by Diverse Compounds. Cell Chemical Biology, 2016, 23, 769-781.	5.2	80
41	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
42	Biochemical and Cellular Characterization and Inhibitor Discovery of Pseudomonas aeruginosa 15-Lipoxygenase. Biochemistry, 2016, 55, 3329-3340.	2.5	39
43	Modelling the Tox21 10â€‰K chemical profiles for in vivo toxicity prediction and mechanism characterization. Nature Communications, 2016, 7, 10425.	12.8	202
44	A potent and selective inhibitor targeting human and murine 12/15-LOX. Bioorganic and Medicinal Chemistry, 2016, 24, 1183-1190.	3.0	15
45	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
46	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
47	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
48	Concise Review: Modeling Central Nervous System Diseases Using Induced Pluripotent Stem Cells. Stem Cells Translational Medicine, 2014, 3, 1418-1428.	3.3	21
49	Identification of ML251, a Potent Inhibitor of T. brucei and T. cruzi Phosphofructokinase. ACS Medicinal Chemistry Letters, 2014, 5, 12-17.	2.8	27
50	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
51	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
52	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
53	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
54	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

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55	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
56	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
57	A Robotic Platform for Quantitative High-Throughput Screening. Assay and Drug Development Technologies, 2008, 6, 637-657.	1.2	126
58	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